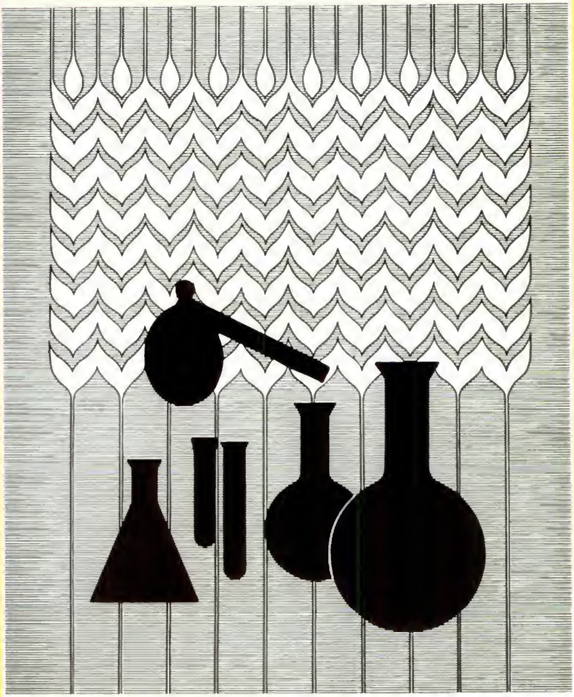
ISSN 0254-4725

Compendium of food additive specifications

Addendum 8

FAO
FOOD AND
NUTRITION
PAPER

52
Add. 8



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Joint FAO/WHO Expert Committee
on Food Additives
55th session
Geneva, Switzerland, 6-15 June 2000

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FIAT PANIS

Rome, 2000

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ISBN 92-5-104508-9

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INTRODUCTION

This volume contains specifications of identity and purity prepared at the fifty-third meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), held in Geneva, 6-15 June 2000. These specifications should be considered only in conjunction with the Report of the above meeting which will be printed in the WHO Technical Report Series. Toxicological monographs of the substances considered at the 55th meeting of JECFA will be published in the WHO Food Additives Series as No. 46.

The general principles applied in the elaboration of specifications established at the earlier JECFA sessions have been published in the Principles for the Safety Assessment of Food Additives and Contaminants in Food, WHO Environmental Health Criteria, No. 70, 1987. The specifications of identity and purity of food additives established by JECFA are meant to identify the substance that has been subject to biological testing, to ensure that the substance is of adequate degree of purity for safe use in food, and to reflect and encourage good manufacturing practices. These principles were last reaffirmed by the 39th session of JECFA in 1992.

The specifications are mainly established for the use of toxicologists and others concerned with the identity and purity of the substance. As agreed by JECFA at its twenty-sixth meeting, specifications may also be established prior to the eventual completion of toxicological evaluation, in certain cases, when the available toxicological data are inadequate or incomplete, and do not permit the establishment of full or temporary acceptable daily intakes (ADIs). References are made in individual specifications to some of the criteria that may be of interest in commerce, but they do not necessarily include all the requirements of interest to the commercial user. These specifications are not more stringent than is necessary to accomplish their purpose and should easily be attainable by the producing industries. The report of the twenty-third session gives the reasons why certain specifications are designated as "tentative".

There were a total of 382 specifications (38 food additives, uses other than flavouring agent; 344 flavouring agents) prepared at the 55th session of which 125 were new. Eighty-five specifications were designated as tentative, and additionally 56 non-tentative specifications for flavouring agents, for which the minimum assay figures were less than 95%, were reclassified as tentative. Sixteen specifications were withdrawn. These compounds are: acetone peroxides, aluminum sodium sulfate, ammonium persulfate, benzoin gum, calcium iodate, calcium peroxide, carbohydrase from *Aspergillus niger*, var., carbohydrase from *Aspergillus awamori*, var., chlorine dioxide, isoamyl gallate, lipase from *Aspergillus oryzae*, var., 2-nitropropane, potassium persulfate, rennet from *Endothia parasitica*, and trichloroethylene.

Comments and suggestions regarding this Volume are encouraged. Please send to Chief, Food Quality and Standards Service, Food and Nutrition Division, FAO, Viale delle Terme di Caracalla, 00100 Rome, Italy.

NOTE: Use of (FNP 5) in specifications refers to General Methods (Guide to JECFA Specifications), FAO Food and Nutrition Paper 5/Rev. 2 (1991).

This One
NT07-Q1H-3EL9

ACKNOWLEDGEMENTS

The Committee wishes to thank Dr. A. Okiyama, visiting scientist, FAO, for his assistance in the preparation of the compendium.

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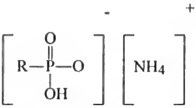
AMMONIUM SALTS OF PHOSPHATIDIC ACID

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 17th JECFA (1973) and published in FNP 4 (1978) and in FNP 52 (1992). An ADI of 0-30 mg/kg bw was established at the 18th JECFA (1974).

SYNONYMS	Ammonium phosphatides, Emulsifier YN, Mixed ammonium salts of phosphorylated glycerides; INS No. 442
DEFINITION	The product consists essentially of a mixture of the ammonium compounds of phosphatidic acids derived from the edible fat (usually partially hardened rapeseed oil). A mono- or diglyceride moiety may be attached to phosphorus. Moreover, two phosphorus esters may be linked together as phosphatidyl phosphatides. The product is prepared by glycerolysis of the fat, followed by phosphorylation with phosphorus pentoxide, and neutralization with ammonia. The article of commerce may be further specified as to water content, hexane-insoluble matter, inorganic hexane-insoluble matter, pH value and triglyceride content.
Structural formula (approximate composition)	 where R may be a mono- or diglyceride moiety
Assay	The phosphorus content is not less than 3.0% and not more than 3.4% by weight; the ammonium N content is not less than 1.2% and not more than 1.5%.
DESCRIPTION	Unctuous semisolid
FUNCTIONAL USES	Emulsifier
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, partially soluble in ethanol and in acetone, soluble in fats
Test for phosphate	Passes tests See description under TESTS
Test for fatty acid	Passes tests See description under TESTS
Test for glycerol (FNP 5)	Passes test
PURITY	
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP5, "Instrumental Methods".

TESTS

IDENTIFICATION TESTS

Test for phosphate

Ignite 1 g of the sample with 2 g of anhydrous sodium carbonate. Cool and dissolve the residue in 5 ml of water and 5 ml of nitric acid. Add 5 ml of ammonium molybdate TS and heat to boiling. A yellow precipitate is obtained.

Test for fatty acid

Reflux 1 g of the product for 1 h with 25 ml of 0.5 N ethanolic potassium fatty acid hydroxide. Ammonia is evolved from the end of the reflux condenser, recognizable by its odour and by its reaction on moist, red litmus paper. On cooling the residue to 0°, a precipitate of potassium soap is obtained.

METHOD OF ASSAY

Determination of phosphorus

Absorption spectrophotometry

Reagents

- Vanadate-molybdate solution: Separately dissolve in water 20 g of ammonium molybdate and 1 g of ammonium vanadate. Mix the two solutions, add 140 ml of concentrated nitric acid and dilute to 1000 ml with water. Mix well.
- Standard phosphate solution: Stock solution: Dissolve 3.8346 g of potassium dihydrogen phosphate, previously dried at 110°, in water and dilute to 1000 ml; 1 ml of this solution = 2.0 mg P_2O_5.

Working solutions

- Sulfuric acid: sp gr 1.84
- Nitric acid: sp gr 1.42
- Perchloric acid: 60%, sp gr 1.54
- Standard phosphate working solution: Transfer 50.0 ml of the standard phosphate solution (1ml = 2.0 mg P_2O_5) to a 500 ml volumetric flask and dilute to volume with water and mix well. 1 ml of standard phosphate working solution = 0.2 mg equivalents of P_2O_5

Procedure

Weigh accurately 1.5 to 1.6 g of a representative sample into a small glass capsule and transfer to a 300-ml Kjeldahl flask containing 5 ml of sulfuric acid and 10 ml of nitric acid. Heat the flask, gently at first, with continual swirling, and later more strongly over a bare flame. Add further measured amounts of nitric acid from time to time, cooling the flask prior to addition, and continue the heating until the stage where the digest is clear and assumes a golden colour. Cool, add 5 ml of 60% perchloric acid and continue the oxidation until white acid fumes form in the flask. Cool again and add 5 ml of water and continue heating until white fumes are again driven off. Cool, dilute carefully with water, cool again and transfer quantitatively to a 500-ml volumetric flask. Dilute to volume with water and mix well (Test solution).

Carry out a blank digestion exactly as above but omit the sample and use the same volume of acid as required to wet oxidize the sample (Blank digest solution).

Into separate 100-ml volumetric flasks, add by burette:

(a) 25.0 ml of Standard phosphate working solution (= 5.0 mg P_2O_5),
(b) 30.0 ml of Standard phosphate working solution (= 6.0 mg P_2O_5),
(c) a 25 ml aliquot of the test solution which will contain the equivalent of between 5 and 6 mg P_2O_5

Into each of the flasks containing the phosphorus standards, i.e. (a) and (b), transfer an aliquot of the blank digest solution equal in volume to (c), in order to compensate for possible traces of phosphorus derived from the acid digest reagents and which may be present in the Test Solution.

To each add 25 ml of the vanadate-molybdate reagent, mix, dilute to nearly 100 ml with

water, mix well, adjust the temperature of the solution to 20°, dilute to the mark with water and re-mix.
After 10 min measure the absorbance of both the 6 mg P_2O_5 solution and the test solution against the 5 mg standard contained in the blank cell. Use optically matched 1 cm cells and measure at a wavelength of 420 nm, or with an Ilford 604 filter if using a photo-electric colorimeter.

Calculation

$$\% \text{ Phosphorus} = [5 + \frac{\text{A test}}{\text{A 6 mg}}] \times \frac{0.873}{W}$$

where

A test = absorbance difference between the 5 mg standard and the test solution
A 6 mg = absorbance difference between the 6 mg and 5 mg standards
W = weight of sample taken (g)

Determination of ammonium nitrogen

Apparatus for steam distillation

The apparatus consists of a 2-L flask fitted with a rubber bung through which pass an approximately 3" length of glass tubing, arranged so that the lower end is near the bottom of the flask, and a shorter L-shaped piece of tubing arranged such that the tube projects about 1/4" below the lower surface of the bung, to act as a steam outlet tube. The flask should be approximately 2/3 filled with distilled water made slightly acid with dilute sulfuric acid TS and contain a few pieces of sintered glass to prevent bumping when the contents of the flask are vigorously boiled to act as a steam generator. A tap funnel may be fitted to the flask if desired to facilitate replenishing the water in the flask between determinations.
The steam outlet tube is connected via a condensation trap to the inlet of a steam distillation head, fitted to a short necked 1-L round bottomed B34 necked flask. The distillation head should be such that the steam inlet tube reaches almost to the bottom of the 1-L flask and the outlet should be fitted with two splash traps, one near the top of the 1-L flask and the other near the top of B19 jointed verticle, single-surface condenser to which the distillation head connects. The vertical condenser should be fitted with an extended outlet tube, able to reach to the bottom of a 500-ml conical flask.

Reagents

- Boric acid solution (2% w/v in water)
- Sodium hydroxide solution (40 w/v in water)
- 0.02N Hydrochloric acid
- Mixed indicator: Mix 5.0 of 0.1% w/v alcoholic solution of bromocresol green and 2.0 of a 0.1% w/v alcoholic solution of methyl red and dilute the mixture to 30 ml with 95% alcohol.
- Silicone fluid 200/50 MS

Procedure

Assemble and thoroughly steam out the apparatus. Accurately weigh about 0.2 g of a representative sample of neutral Ammonium salts of phosphatidic acids into a small glass phial (approx. 3/4" diameter, 1/2" deep). Transfer the phial and weighed contents to the distillation flask and add approximately 250 ml distilled water. Connect the distillation head and splash traps to the distillation flask and vertical condenser, and arrange the condenser such that the outlet dips below the surface of 10 ml of 2% boric acid and 1 ml mixed indicator contained in a 500-ml conical flask. Add to the distillation flask, via a funnel attached by means of a short piece of rubber tubing to the steam inlet tube, 75 ml 40% aqueous sodium hydroxide, and wash in with distilled water. Detach the funnel and connect the steam inlet to the steam supply. (Alternatively, the sodium hydroxide may be added to the flask through a tap funnel, fitted to the distillation flask if preferred and washed in with distilled water. If so a liquid seal should be maintained in the funnel during the addition and distillation). Vigorously steam distil the contents of the distillation flask and collect

200 ml distillate in the boric acid. During the distillation gently agitate the distillation flask if necessary, to avoid the sample being deposited around the upper surfaces of the flask. When the required amount of distillate has been collected, lower the receiving flask, stop the steam supply, and wash down the inside of the condenser, and the outside of the lower end, with a small quantity of distilled water, collecting the washings in the receiving flask. Titrate the contents of the receiving flask with 0.02N hydrochloric acid. Carry out at least one blank determination in exactly the same way but omitting the sample.

During the distillation difficulty may be experienced with frothing of the contents of the distillation flask. If so, 2 drops of silicone fluid should be added to the distillation flask at the time of adding the sample; and a similar amount included in the blank determination.

Calculation

1 ml of 0.02 N HCl = 0.2802 mg of nitrogen.

$$\% \text{ Nitrogen} = \frac{(\text{sample titre} - \text{blank titre}) \text{ x } 28.02}{(\text{sample wt. in mg})}$$

α-AMYLASE AND GLUCOAMYLASE FROM *ASPERGILLUS ORYZAE*, VAR.

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 41st JECFA (1993) and published in FNP 52 Add 2 (1993). An ADI was "Acceptable" established at the 31st JECFA (1987).

SYNONYMS	INS No. 1100
SOURCES	Produced by the controlled fermentation of non-toxicogenic and non-pathogenic strains of *Aspergillus oryzae* and isolated from the growth medium.
ACTIVE PRINCIPLES	α-Amylase (synonyms: diastase, ptyalin, glycogenase) Glucan 1,4-α-glucosidase (synonyms: amyloglucosidase, acid maltase, lysosomal α-glucosidase, exo-1,4-α-glucosidase)
SYSTEMATIC NAMES AND NUMBERS	1,4-α-D-Glucan glucanohydrolase (EC 3.2.1.1) 1,4-α-D-Glucan glucohydrase (EC 3.2.1.3)
REACTIONS CATALYZED	α-Amylase hydrolyzes 1,4-α-glucosidic linkages in polysaccharides yielding dextrins, oligosaccharides and glucose. Glucoamylase hydrolyzes 1,4-α- and 1,6-α-glucosidic linkages in polysaccharides yielding glucose.
SECONDARY ENZYME ACTIVITIES	Lipase (EC 3.1.1.3) Tannase (EC 3.1.1.20) Cellulase (EC 3.2.1.4) Endo-1,3-β-glucanase (EC 3.2.1.6) Pectinase (EC 3.2.1.15) Maltase (EC 3.2.1.20) Lactase (EC 3.2.1.23) Endo-1,4-β-mannanase (EC 3.2.1.78) Protease
DESCRIPTION	Typically tan amorphous powders or tan to dark-brown liquids that may be dispersed in food-grade diluents and may contain stabilizers and preservatives; soluble in water and practically insoluble in ethanol and ether.
FUNCTIONAL USES	Enzyme preparation Used in the hydrolysis of cereals and starch; in the preparation of fruit and vegetable products, beverages, sugar, confectionery and bakery products; and in honey.
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7).

CHARACTERISTICS

IDENTIFICATION

α-Amylase activity (FNP 5)	The sample shows fungal α-amylase activity
Glucoamylase activity (FNP 5)	The sample shows fungal glucoamylase activity

α-AMYLASE FROM *ASPERGILLUS ORYZAE*, VAR.

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Acceptable" was established at the 31st JECFA (1987).

SYNONYMS	INS No. 1100
SOURCES	Produced by the controlled fermentation of non-toxicogenic and non-pathogenic strains of *Aspergillus oryzae* and isolated from the growth medium
ACTIVE PRINCIPLES	α-Amylase (synonyms: diastase, ptyalin, glycogenase)
SYSTEMATIC NAMES AND NUMBERS	1,4-α-D-Glucan glucanohydrolase (EC 3.2.1.1)
REACTIONS CATALYZED	The enzyme preparations hydrolyze 1,4-α-glucosidic linkages in polysaccharides, yielding dextrins and oligo- and monosaccharides.
SECONDARY ENZYME ACTIVITIES	Amyloglucosidase Proteases Xylanase
DESCRIPTION	Typically tan amorphous powders or tan to dark-brown liquids that may be dispersed in food-grade diluents and may contain stabilizers and preservatives; soluble in water and practically insoluble in ethanol and ether.
FUNCTIONAL USES	Enzyme preparation Used in starch hydrolysis, syrup production, baking and brewing
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7)
CHARACTERISTICS	
IDENTIFICATION	
α-Amylase activity (FNP 5)	The sample shows fungal α-amylase activity

AMYLOGLUCOSIDASE FROM *ASPERGILLUS NIGER*, VAR.
(Tentative)

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Not specified" was established at the 35th JECFA (1989).

Information required on the assay of amyloglucosidase in formulated products containing glucose. Comments on other aspects of the monograph are invited.

SYNONYMS INS No. 1100

SOURCES Produced by the controlled fermentation of non-pathogenic and non-toxicogenic strains of *Aspergillus niger*, isolated from the growth medium.

ACTIVE PRINCIPLES Glucan 1,4-α-glucosidase (synonyms: glucoamylase, acid maltase, lysosomal α-glucosidase, exo-1,4-α-glucosidase)

SYSTEMATIC NAMES AND NUMBERS 1,4-α-D-Glucan glucohydrase (EC 3.2.1.3; C.A.S. No. 9032-08-0)

REACTIONS CATALYZED Hydrolyzes 1,4-α, 1,6-α and 1,3-α glucosidic linkages to yield glucose.

SECONDARY ENZYME ACTIVITIES α-Amylase (1,4-α-D-Glucan-glucanohydrolase; EC 3.2.1.1; C.A.S. No. 9000-90-2).

Cellulase ((1,4-[1,3; 1,4]-β-D-Glucan 4-glucano-hydrolase; EC 3.2.1.4; C.A.S. No. 9012-54-8)

DESCRIPTION Typically off-white to tan amorphous powders or tan to dark-brown liquids. The unformulated products are concentrated and standardised with food-grade diluents or carriers and may contain stabilizers as glycerol and preservatives as sodium benzoate or as the dried powder form with food grade sucrose or glucose. Soluble in water and practically insoluble in ethanol and ether.

FUNCTIONAL USES Enzyme preparation

Used to convert starches to carbohydrates in the preparation of starch syrups, dextrose, fruit juices and cheese.

GENERAL SPECIFICATIONS Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7).

CHARACTERISTICS

IDENTIFICATION

Amyloglucosidase activity The sample shows amyloglucosidase activity.

See description under TESTS

TESTS

Amyloglucosidase activity

Principle

This method applies to unformulated or formulated products without glucose. The method is based on the ability of the enzyme to hydrolyze maltose to glucose. The formed glucose is converted to gluconolactone by glucose dehydrogenase in the presence of NAD^+ that is converted to NADH. The change in the concentration of NAD^+ is measured photometrically at 340 nm. One amyloglucosidase unit (AGU) is defined as the amount of enzyme that cleaves 1 µmol of maltose per minute under standard assay conditions (substrate concentration 10 mg/ml; temperature 37.0 °; pH 5.0; incubation time 30 min).

Apparatus:
Spectrophotometer set at 540 nm.
Vortex mixer
Water bath set at 37.0 ± 0.1 °.

Reagents and solutions:
Maltose substrate:
Dissolve 1000 mg maltose (Merck N° M5912 or equivalent) in 0.1 M citrate buffer, pH 5.0, making a total volume of 50 ml (to be prepared each day of analysis).

Glucose dehydrogenase (GluDH) reagent:
Add buffer solution (Merck No. 14051 or equivalent) to the enzyme mixture (Merck No. 14055, bottles "1" and "2", or equivalent). Allow the mixture to stand for 15 min. Transfer the solution to a 500 ml volumetric flask, containing 200 ml of 0.1 M citrate buffer pH 5.0. Fill the flask to the mark with the same buffer. This solution can be stored for two weeks at room temperature (not in a refrigerator).

Preparation of standard enzyme solutions:
Dilute an amyloglucosidase standard (Sigma A-7420 or equivalent) with known activity in 10 mM NACl to give the following enzyme units per ml: 0.015, 0.030, 0.045, 0.060 and 0.075.

Procedure

Measurement of enzyme activity:
Add 500 µl of substrate solution (20 mg/ml maltose, prepared in 0.1 M citrate buffer, pH 5.0, pre-warmed to 37 °) to an equal volume of enzyme solution also pre-warmed to 37 °. Mix the resulting solution thoroughly and transfer to a water bath maintained at 37.0 °. After 30 minutes remove the test tube from the water bath, and add 1000 µl of the stop reagent (0.06 N NaOH) and shake vigorously. Add 3 ml of GluDH reagent and mix again. Leave the test tube at room temperature for exactly 30 min and measure absorbance (A) at 340 nm. Prepare a blank in a similar manner except that the stop reagent is added before the substrate.

Calculation of enzyme activity:
Draw the enzyme standard curve in a coordinate system using enzyme activity (AGU/ml) as the abscissa and ΔA (sample-blank) as the ordinate. Calculate the activity of the sample by reading ΔA of sample dilutions on the standard curve and then multiplying by the corresponding dilution factors. The standard curve is a straight line passing through the origin and linear regression can therefore be applied.

Basic standardisation:
Glucose solutions:
a) Stock solution: Accurately weigh 1.60 g of glucose, analytical grade, in a 1000 ml volumetric flask and make up to volume with water.
b) Standard solutions: Dilute 1.0, 2.0, 3.0, 4.0, 5.0 and 6.0 ml of stock solution to volume with water in 100-ml volumetric flask to give standard solutions of 88.8, 178, 266, 355, 444 and 533 µmol.

Standard curve:
Prepare the glucose standard curve by mixing 2.0 ml glucose solution with 3.0 ml GluDH reagent and incubating at room temperature for 30 min. Read A at 340 nm. Prepare a common blank using water instead of glucose solution. Plot glucose concentration (µmol/1) versus ΔA.

Calculation:
Calculate the enzyme activity (AGU/g) by reading the equivalent glucose concentration on the standard curve and inserting it in the following formula:

$$\text{AGU/g} = \frac{A \times 4 \times F}{30 \times 1000}$$

Where:

A = reading on the standard curve, µmol/l
F = dilution factor of the enzyme solution, ml/g
4 = the ratio between amount of enzyme dilution in sample and amount of glucose solution in standard
30 = incubation time, 30 min
1000 = conversion from liter to ml

ALUMINIUM POTASSIUM SULFATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 22nd JECFA (1978) and published in FNP 7 (1978) and in FNP 52 (1992). No ADI was allocated at the 22nd JECFA (1978).

SYNONYMS	Potassium alum, potash alum Burnt alum (anhydrous) INS No. 522 (dodecahydrate)

DEFINITION

Chemical names	Aluminium potassium sulfate dodecahydrate Aluminum potassium sulfate anhydrous
C.A.S. number	7784-24-9 (dodecahydrate) 10043-67-1 (anhydrous)
Chemical formula	$AlK(SO_4)_2 \cdot xH_2O$ (x = 0 or 12)
Formula weight	474.38 (dodecahydrate) 258.21 (anhydrous)
Assay	Dodecahydrate: not less than 99.5% Anhydrous form: not less than 96.5%
DESCRIPTION	Large, transparent crystals or crystalline fragments, or white crystalline powder; odourless
FUNCTIONAL USES	Acidity regulator, firming agent, raising agent

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)	Freely soluble in water; insoluble in ethanol
pH (FNP 5)	3.0 - 4.0 (10% soln)
Test for aluminium (FNP 5)	Passes test
Test for sulfate (FNP 5)	Passes test
Test for potassium (FNP 5)	Passes test

PURITY

Ammonium salts	Heat 1 g of the sample with 10 ml of sodium hydroxide TS on a steam bath for 1 min. The odour of ammonia is not perceptible.
Fluoride	Not more than 30 mg/kg See description under TESTS
Lead	Not more than 3 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods"

TESTS

PURITY TESTS

Fluoride

Lime Suspension: Carefully slake about 56 g of low-fluoride calcium oxide (about 2 mg/kg F) with 250 ml of water, and add 250 ml of 60% perchloric acid slowly and with stirring. Add a few glass beads, and boil to copious fumes of perchloric acid, then cool, add 200 ml of water, and boil again. Repeat the dilution and boiling once more, cool, dilute considerably, and filter through a fritted glass filter, if precipitated silicon dioxide appears. Pour the clear solution, with stirring, into 1000 ml of a 1 in 10 sodium hydroxide solution, allow the precipitate to settle, and siphon off the supernatant liquid. Remove the sodium salts from the precipitate by washing 5 times in large centrifuge bottles, shaking the mass thoroughly each time. Finally, shake the precipitate into a suspension and dilute to 2000 ml. Store in paraffin-lined bottles and shake well before use. 100 ml of this suspension should give no appreciable fluoride blank when evaporated in a platinum dish and treated as directed below under "Procedure", beginning with "Ignite briefly at 600°,...".

Distillation Apparatus: Connect a 125-ml distillation flask with a condenser. Equip also with a thermometer and a capillary tube, both of which must extend into the liquid. Connect a small dropping funnel or a steam generator to the capillary tube. Support the flask on an asbestos mat with a hole which exposes about one-third of the flask to the flame. To minimize the distillation blank resulting from fluoride leached from the glassware, the distillation apparatus should be treated as follows: treat the glassware with hot 10% sodium hydroxide solution, followed by flushing with tap water and rinsing with distilled water. At least once daily, treat in addition by boiling down 15-20 ml of a 1 in 2 sulfuric acid solution until the still is filled with fumes; cool, pour off the acid, treat again with 10% sodium hydroxide solution, and rinse thoroughly.

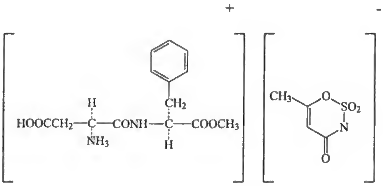
Procedure: Add to the distilling flask 1.67 g of the sample, accurately weighed, and 25 ml of a 1 in 2 sulfuric acid solution. Distil until the temperature reaches 160°, then maintain at 160° to 165° by adding water from the funnel, collecting 300 ml of distillate. Oxidize the distillate by the cautious addition of 2 or 3 ml of fluoride-free 30% hydrogen peroxide (to remove sulfites), allow to stand for a few min, and evaporate in a platinum dish with an excess of Lime Suspension. Ignite briefly at 600°, then cool and wet the ash with about 10 ml of water. Cover the dish with a watch glass, and cautiously introduce under cover just sufficient 60% perchloric acid to dissolve the ash. Add the contents of the dish through the dropping funnel of a freshly treated distilling apparatus (the distilling flask should contain a few glass beads), using a total of 20 ml of 60% perchloric acid for dissolving the ash and transferring the solution. Add 10 ml of water and a few drops of a 1 in 2 silver perchlorate solution through the dropping funnel. Continue as directed in the Limit Test, Method I. *Thorium Nitrate Colorimetric Method*, beginning with "Distil until the temperature reaches 135° ...".

METHOD OF ASSAY

Weigh accurately about 4 g of the sample, transfer into a 250-ml volumetric flask. Dissolve in water, dilute to volume with water, and mix. Pipet 10 ml of this solution into a 250-ml beaker, add 25.0 ml of 0.05 M disodium ethylenediaminetetra-acetate, and boil gently for 5 min. Cool, and with continuous stirring add in the order given: 20 ml of pH 4.5 buffer solution (77.1 g of ammonium acetate and 57 ml of glacial acid in 1000 ml), 50 ml of ethanol, and 2 ml of dithizone TS. Titrate with 0.05 M zinc sulfate until the colour changes from green-violet to rose-pink, and perform a blank determination, substituting 10 ml of water for the sample. Each ml of 0.05 M disodium ethylenediaminetetraacetate is equivalent to 8.553 mg of $Al_2(SO_4)_3$.

ASPARTAME-ACESULFAME SALT

New specifications prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000). The aspartame and acesulfame moieties are covered by the ADIs for aspartame (0-40 mg/kg bw) established at the 25th JECFA (1981) and for acesulfame K (0-15 mg/kg bw) established at the 37th JECFA (1990).

SYNONYMS	Aspartame-acesulfame
DEFINITION	The salt is prepared by heating an approximately 2:1 ratio (w:w) of aspartame and acesulfame K in solution at acidic pH and allowing crystallization to occur after adjusting the pH to alkalinity. The potassium and moisture are eliminated. The product is more stable than aspartame alone.
Chemical names	The 6-methyl-1,2,3-oxathiazine-4(3H)-one-2,2-dioxide salt of L-phenylalanyl-2-methyl-L-α-aspartic acid.
C.A.S. number	106372-55-8
Chemical formula	$C_{18}H_{23}O_9N_3S$
Structural formula	 + - H CH₂ HOOCCH₂—C—CONH—C—COOCH₃ NH₃ H CH₃ O SO₂ N O
Formula weight	457.46
Assay	63.0% to 66.0% aspartame (dry basis) and 34.0% to 37.0% acesulfame (acid form on a dry basis).
DESCRIPTION	A white, odourless, crystalline powder.
FUNCTIONAL USES	Sweetening agent, flavour enhancer
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Slightly soluble in water and ethanol.
PURITY	
Loss on drying (FNP 5)	No more than 0.5% (105°, 4 h)
Transmittance (FNP 5)	The transmittance of a 1% solution in water determined in a 1 cm cell at 430 nm with a suitable spectrophotometer using water as a reference, is not less than 0.95, equivalent to an absorbance of not more than approximately 0.022.
Specific Rotation (FNP 5)	$[\alpha]_D^{20}$+14.5 to +16.5. Determine at a concentration of 6.2 g in 100 ml formic acid (15N) within 30 min of

preparation of the solution. Divide the calculated specific rotation by 0.643 to correct for the aspartame content of the aspartame-acesulfame salt.

5-Benzyl-3,6-dioxo-2-piperazineacetic acid

Not more than 0.5%
See description under TESTS

Lead

Not more than 1 mg/kg.
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods."

TESTS

PURITY TESTS

5-Benzyl-3,6-dioxo- 2-piperazine acetic acid

Principle: Aspartame-acesulfame salt is dissolved in methanol-water and the 5-benzyl-3,6-dioxo-2-piperazine acetic acid determined by comparison to an authentic standard after separation by HPLC.
Apparatus: Use a suitable high-pressure liquid chromatograph equipped with UV detector measuring absorbance at 210 nm and a 250 x 4.6 mm column packed with octyldecyl silanized silica (10-µm Partisil ODS-3 or equivalent) and operated under isocratic conditions at 40°.
Mobile phase: Dissolve 5.6 g of potassium phosphate monobasic into 820 ml of water in a 1-l flask and adjust the pH to 4.3 with phosphoric acid. Add 180 ml of methanol and mix. Filter through a 0.45 µm filter and de-gas.
Standard: Accurately weigh approximately 25 mg of authentic 5-benzyl-3,6-dioxo- 2-piperazine acetic acid into a 100-ml volumetric flask and dilute to volume with water and mix. Accurately transfer 15 ml of this solution to a 50-ml flask and dilute to volume with a 1:9 (v:v) mixture of methanol:water.
Sample: Accurately weigh approximately 50 mg of sample into a 10 ml volumetric flask and dilute to volume with a 1:9 (v:v) mixture of methanol:water.
Procedure: Separately inject 20 µl portions of the standard and the sample into the chromatograph and record the peak areas in standard and sample chromatograms (under the conditions described, the retention time of 5-benzyl-3,6-dioxo-2-piperazine acetic acid and aspartame are approximately 4 and 11 min, respectively). Calculate the percentage of 5-benzyl-3,6-dioxo-2-piperazine acetic acid as follows:

$\% = 1000(A_U C_S)/(A_S W_u)$

Where: A_U and A_S are the peak areas of 5-benzyl-3,6-dioxo-2-piperazine acetic acid in the sample and standard, respectively, C_S is the concentration of 5-benzyl-3,6-dioxo- 2-piperazine acetic acid in the standard in mg/ml and W_u is the weight, in mg, of aspartame-acesulfame salt taken in the sample preparation.

METHOD OF ASSAY

Principle: Aspartame-acesulfame salt is dissolved in methanol and potentiometrically titrated with tetrabutylammonium hydroxide.
Apparatus: Use an suitable autotritator (e.g. Metrohm 670, or equivalent) equipped with a glass pH electrode with a silver-silver chloride double liquid junction reference electrode (e.g., Yokogawa pH electrode SM 21-AL4 or equivalent and reference electrode SR 20-AS52 or equivalent).

Standardize a fresh solution of tetrabutylammonium hydroxide by preparing a 0.1 M solution in a 1:1 (v:v) mixture of 2-propanol:methanol. Weigh 24 and 98 mg benzoic acid with 0.01 mg accuracy and dissolve each into two 50-ml volumetric flasks and dilute to volume with 2-propanol. Titrate both solutions with the 0.1 M tetrabutylammonium hydroxide and record the volume required to reach the equivalence point with 0.001 ml accuracy. Perform a blank titration on 50 ml of 2-propanol. Determine the standard factor (F) for each titration. and average the two factors as follows:

$F = [(W_S \times 1000)/(122 \times (V_S - V_O))]$

Where

W_S = weight of primary benzoic acid in g
V_S = volume of equivalence point in ml
V_o = volume of equivalence for the blank in ml
122 = molecular weight of benzoic acid

Assay: Weigh accurately 100 to 150 mg aspartame-acesulfame salt and dissolve in 50-ml methanol and titrate with the above standardized 0.1 M tetrabutylammonium hydroxide. Determine the volume (ml) of standard solution to reach the first (V1)and second (V2) equivalency points. Perform a blank titration on the methanol. Calculate the acesulfame and aspartame content as follows:

Acesulfame content (% m/m) = $[(V_1\text{-}V_B) \times N \times 163/(10 \times W)]$

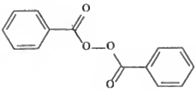
Aspartame content (% m/m) = $[(V_2\text{-}V_1) \times N \times 294/(10 \times W)]$

Where

W = Weight of sample in g
V_1 = volume of first equivalence point of sample in ml
V_2 = volume of second equivalence point of sample in ml
V_B = volume of equivalence point of blank in ml
N = normality of the standard 0.1 M tetrabutylammonium hydroxide (see above)
163 and 294 = formula weights of acesulfame and aspartame moieties, respectively
10 = conversion of g to % (m/m)

BENZOYL PEROXIDE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 19th JECFA (1975), published in NMRS 55B (1976) and in FNP 52 (1992). The 7th JECFA (1963) had insufficient data to establish an ADI, but noted that the evidence permitted an estimate of an acceptable level of treatment of 0 - 40 mg/kg of flour for human consumption (conditional acceptance for special purposes: 40-75 mg/kg).

SYNONYMS	Benzoyl superoxide, INS No. 928
DEFINITION	
Chemical names	Dibenzoyl peroxide
C.A.S. number	94-36-0
Chemical formula	$C_{14}H_{10}O_4$
Structural formula	
Formula weight	242.23
Assay	Not less than 96.0%
DESCRIPTION	Colourless, crystalline solid having a faint odour of benzaldehyde. Caution: Benzoyl peroxide is a highly reactive compound and may give rise to explosions
FUNCTIONAL USES	Flour treatment agent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, slightly soluble in ethanol, soluble in ether
Melting range (FNP 5)	103 - 106° with decomposition
Decomposition to benzoic acid	To 0.5 g of the sample peroxide add 50 ml of 0.5 N ethanolic potassium hydroxide, heat gradually to boiling and continue boiling for 15 min. Cool and dilute with 200 ml of water. Add sufficient 0.5 N hydrochloric acid to make strongly acidic and extract with ether. Dry the ether solution over anhydrous sodium sulfate, and then evaporate to dryness on a steam bath. The residue of benzoic acid so obtained melts between 121° and 123°.
PURITY	
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

METHOD OF ASSAY

Dissolve about 250 mg of the sample, accurately weighed, in 15 ml of acetone in a 100-ml glass-stoppered bottle. Add 3 ml of 50% (w/v) potassium iodide solution and swirl for 1 min. Titrate immediately with 0.1 N sodium thiosulfate (without addition of starch as an indicator). Each ml of 0.1 N sodium thiosulfate is equivalent to 12.11 mg of $C_{14}H_{10}O_4$.

BLACKCURRANT EXTRACT
(Tentative)

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 30th JECFA (1986), published in FNP 37 (1986) and in FNP 52(1992). No ADI was established.

Information required on the chromatographic identification test and adequacy of sample size for the sulfur dioxide test. Comments on other aspects of the monograph are invited.

SYNONYMS

INS No. 163(iii)

DEFINITION

Blackcurrant extract is obtained from blackcurrant pomace by aqueous extraction. The main colouring principles are four anthocyanins (cyanidin 3-rutinoside, delphinidin 3-rutinosid, cyanidin 3-glucoside, delphinidin 3-glucoside). Most of the extracted sugars are fermented to alcohol and practically all the alcohol is removed during the concentration of extract by vacuum evaporation. During the extraction process, sulfur dioxide is used and residual sulfur dioxide may be present. Maltodextrin may be added and the product spray dried.

Chemical names

I. Cyanidin 3-rutinoside
II. Delphinidin 3-rutinoside
III. Cyanidin 3-glucoside
IV. Delphinidin 3-glucoside

C.A.S. number

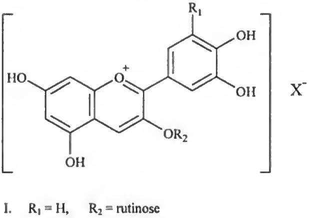
I. 18719-76-1
II. 15674-58-5
III. 7084-24-4
IV. 6906-38-3

Chemical formula

I. $[C_{27}H_{31}O_{15}]^+ X^-$
II. $[C_{27}H_{31}O_{16}]^+ X^-$
III. $[C_{21}H_{21}O_{11}]^+ X^-$
IV. $[C_{21}H_{21}O_{12}]^+ X^-$

Where X^-= counter ion

Structural formula



I. R_1 = H, R_2 = rutinose
II. R_1 = OH, R_2 = rutinose
III. R_1 = H, R_2 = glucose
IV. R_1 = OH, R_2 = glucose

Where X^-= counter ion

Assay

The colour intensity is not less than declared on the label of the product

DESCRIPTION	Purplish-red liquid or powder having a characteristic odour
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Soluble in water and ethanol
Spectrophotometry (FNP 5)	At pH 3 the absorbance maximum is about 520 nm.
Colour reaction	Add 0.1 g of the sample to 50 ml of water and shake thoroughly. Filter if necessary. The solution shows red to purplish-red colour and it turns to blue or dark green on the addition of sodium hydroxide TS.
Chromatography	Information required
PURITY	
Sulfur dioxide	Not more than 50 mg/kg for each unit of colour intensity See description under TESTS and METHOD OF ASSAY
Basic colouring matter	Add 1 g of the sample to 100 ml of 1% sodium hydroxide solution and shake well. Extract 30 ml of this solution with 15 ml ether. Extract the ether solution twice with 5 ml dilute acetic acid TS. The acetic acid extract is colourless.
Other acidic colouring matters	Add 1 ml of ammonia TS and 10 ml of water to 1 g of the sample. Following the directions in Chromatography (FNP 5) place 2 µl of the solution on the chromatographic sheet and dry it. Use a mixture of pyridine and ammonia TS (2:1 by volume) as developing solvent and stop the development when the solvent front reaches about 15 cm height from the point where the sample solution was placed. No spot is observed in daylight at the solvent front after drying. If any spot is observed, it should be decolourized when sprayed with a solution of 40% stannous chloride in hydrochloric acid.
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Method"
TESTS	
PURITY TESTS	
Sulfur dioxide	Distil 1 g of the sample with 100 ml of water and 25 ml of 30% phosphoric acid solution in a distilling flask with the Wagner tube. In an absorption flask, place 25 ml of 2% lead acetate solution previously prepared. Insert the lower end of the condenser into the lead acetate solution in the absorption flask. Distil until the liquid in the absorption flask reaches about 100 ml and rinse the end of the condenser with a little amount of water. To the distilled solution add 5 ml of hydrochloric acid and 1 ml of starch TS, and titrate with 0.01 N iodine. Each ml of 0.01 N iodine is equivalent to 0.3203 mg of SO_2.
METHOD OF ASSAY	Prepare approximately 200 ml of pH 3.0 citric acid dibasic sodium phosphate buffer solution: Mix 159 volumes of 2.1% citric acid solution and 41 volumes of 0.16% dibasic sodium phosphate solution, and adjust the pH to 3.0, using the citric acid solution or dibasic sodium phosphate solution.
	Weigh accurately an adequate amount of the sample so that the measured absorbance is between 0.2 and 0.7, and add pH 3.0 citric acid - dibasic sodium phosphate buffer solution to make up a 100-ml solution. Measure the absorbance A

of this solution in a 1 cm cell at the wavelength of maximum absorption around 520 nm, using pH 3.0 citric acid - dibasic sodium phosphate buffer solution as the blank.

Colour intensity = [A x 10]/[weight of sample (g)]

CARAMEL COLOURS

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 31st JECFA (1987), published in FNP 38 (1988) and in FNP 52 (1992). An ADI for Class I 'Not specified' was established at the 29th JECFA (1985), for Class II of 0-160 mg/kg bw was established at the 55th JECFA (2000) and an ADI for Class III of 0-200 mg/kg bw (0-150 mg/kg bw on solids basis) was established at the 29th JECFA (1985) and an ADI for Class IV of 0-200 mg/kg bw (0-150 mg/kg bw on solids basis) was established at the 29th JECFA (1985).

SYNONYMS

Caramel colours are divided into four classes. The synonyms for each class are:

Class I: Plain caramel, caustic caramel; INS No. 150a
Class II: Caustic sulfite caramel; INS No. 150b
Class III: Ammonia caramel; INS No. 150c
Class IV: Sulfite ammonia caramel , INS No. 150d

DEFINITION

Complex mixtures of compounds, some of which are in the form of colloidal aggregates, manufactured by heating carbohydrates either alone or in the presence of food-grade acids, alkalis or salts; classified according to the reactants used in their manufacture as follows:

Class I: Prepared by heating carbohydrates with or without acids or alkalis; no ammonium or sulfite compounds are used.
Class II: Prepared by heating carbohydrates with or without acids or alkalis in the presence of sulfite compounds; no ammonium compounds are used.
Class III: Prepared by heating carbohydrates with or without acids or alkalis in the presence of ammonium compounds; no sulfite compounds are used.
Class IV: Prepared by heating carbohydrates with or without acids or alkalis in the presence of both sulfite and ammonium compounds.

In all cases the carbohydrate raw materials are commercially available food-grade nutritive sweeteners consisting of glucose, fructose and/or polymers thereof. The acids and alkalis are food-grade sulfuric or citric acids and sodium, potassium or calcium hydroxides or mixtures thereof.

Where ammonium compounds are used they are one or any of the following: ammonium hydroxide, ammonium carbonate and ammonium hydrogen carbonate, ammonium phosphate, ammonium sulfate, ammonium sulfite and ammonium hydrogen sulfite.

Where sulfite compounds are used they are one or any of the following: sulfurous acid, potassium, sodium and ammonium sulfites and hydrogen sulfites.

Food-grade anti-foaming agents may be used as processing aids during manufacture.

DESCRIPTION

Dark brown to black liquids or solids having an odour of burnt sugar

FUNCTIONAL USES

Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)	Miscible with water
Identification of colouring matters (FNP 5)	Passes test
Classification	Class I: Not more than 50% of the colour is bound by DEAE Cellulose and not more than 50% of the colour is bound by Phosphoryl Cellulose.

	Class II: More than 50% of the colour is bound by DEAE Cellulose and it exhibits an Absorbance Ratio of more than 50. Class III: Not more than 50% of the colour is bound by DEAE Cellulose and more than 50% of the colour is bound by Phosphoryl Cellulose. Class IV: More than 50% of the colour is bound by DEAE Cellulose and it exhibits an Absorbance Ratio of not more than 50. See description under TESTS
PURITY	Note: Arsenic and lead metals limits apply to all classes of caramel and are expressed on the basis of the product as is: Other limits and ranges apply to the individual classes as indicated and, unless otherwise stated, are expressed on a solids basis.
Solid content	Class I: 62-77% Class II: 65-72% Class III: 53-83% Class IV: 40-75% See description under TESTS
Colour intensity	Class I: 0.01-0.12 Class II: 0.06-0.10 Class III: 0.08-0.36 Class IV: 0.10-0.60 See description under TESTS
Total nitrogen	Class I: max 0.1% Class II: max 0.2% Class III: 1.3 -6.8% Class IV: 0.5-7.5% Determine as directed under Nitrogen Determination (Kjeldahl Method) using Method II (FNP 5)
Total sulfur	Class I: max 0.3% Class II: 1.3 -2.5% Class III: max 0.3% Class IV: 1.4-10.0% See description under TESTS
Sulfur dioxide	Class I: - Class II: max 0.2% Class III: - Class IV: max 0.5% See description under TESTS
Ammoniacal nitrogen	Class I: - Class II: - ClassIII: max 0.4% Class IV: max 2.8% See description under TESTS
4-Methylimidazole (MEI)	Class I: - Class II: - Class III: max 300 mg/kg & max 200 mg/kg on an equivalent colour basis Class IV: max 1000 mg/kg & max 250 mg/kg on an equivalent colour basis See description under TESTS
2-Acetyl-4-tetrahydroxy-butylimidazole (THI)	Class I: - Class II: - Class III: max 40 mg/kg & max 25 mg/kg on an equivalent colour basis. Class IV: - See description under TESTS

Arsenic (FNP 5)

Not more than 1 mg/kg (Method II)

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental methods".

TESTS

IDENTIFICATION TESTS

Classification/Colour bound by DEAE Cellulose

For the purposes of this specification, colour bound by DEAE cellulose is defined as the percentage of decrease in absorbance of a caramel colour solution at 560 nm after treatment with DEAE Cellulose.

Special reagent: DEAE (diethylaminoethyl) Cellulose of 0.7 meq/gram capacity, e.g. Cellex D from Bio-Rad or equivalent DEAE Celluloses of higher or lower capacities in proportionately higher or lower quantities.

Procedure: Prepare a caramel colour solution of approximately 0.5 absorbance unit at 560 nm by transferring an appropriate amount of caramel colour into a 100-ml volumetric flask with the aid of 0.025 N hydrochloric acid. Dilute to volume with 0.025 N hydrochloric acid and centrifuge or filter, if solution is cloudy. Take a 20 ml aliquot of the caramel colour solution, add 200 mg of DEAE Cellulose, mix thoroughly for several min, centrifuge or filter, and collect the clear supernatant. Determine the absorbance of the caramel colour solution and the supernatant in a 1-cm cell at 560 nm, with a suitable spectrophotometer previously standardized using 0.025 N hydrochloric acid as reference. Calculate the percentage of Colour Bound by DEAE Cellulose by the formula:

$$\frac{(X_1 - X_2)}{X_1} \times 100$$

where
X_1 is the absorbance of the caramel colour solution at 560 nm
X_2 is the absorbance of the supernatant after DEAE Cellulose treatment at 560 nm

Classification/Colour bound by phosphoryl cellulose

For the purposes of this specification colour bound phosphoryl cellulose is defined as the percentage of decrease in absorbance of a caramel colour solution at 560 nm after treatment with Phosphoryl Cellulose.

Special Reagent: Phosphoryl Cellulose of 0.85 meq/gram capacity, e.g. Cellex P from Bio-Rad or equivalent Phosphoryl Celluloses of higher or lower capacities in proportionately higher or lower quantities.

Procedure: Transfer 200-300 mg of caramel colour into a 100-ml volumetric flask, dilute to volume with 0.025 N hydrochloric acid, and centrifuge or filter, if solution is cloudy. Take a 40 ml aliquot of the caramel colour solution, add 2.0 g Phosphoryl Cellulose and mix thoroughly for several min. Centrifuge or filter, and collect the clear supernatant. Determine the absorbance of the caramel colour solution and the supernatant in a 1-cm cell at 560 nm, with a suitable spectrophotometer previously standardized using 0.025 N hydrochloric acid as reference. Calculate the percentage of Colour Bound by Phosphoryl Cellulose by the formula:

$$\frac{(X_1 - X_2)}{X_1} \times 100$$

where
X_1 is the absorbance of the caramel colour solution at 560 nm
X_2 is the absorbance of the supernatant after Phosphoryl Cellulose treatment at 560 nm

Classification/

For the purposes of this specification, Absorbance Ratio is defined as the absorbance of

Absorbance ratio

caramel colour at 280 nm divided by the absorbance of caramel colour at 560 nm.

Procedure: Transfer 100 mg of caramel colour into a 100-ml volumetric flask with the aid of water, dilute to volume, mix and centrifuge if solution is cloudy. Pipet a 5.0 ml portion of the clear solution into a 100-ml volumetric flask, dilute to volume with water, and mix. Determine the absorbance of the 0.1% solution in a 1-cm cell at 560 nm and that of the 1:20 diluted solution at 280 nm with a suitable spectrophotometer previously standardized using water as reference. (A suitable spectrophotometer is one equipped with a monochromator to provide a band width of 2 nm or less and of such quality that the stray-light characteristic is 0.5% or less.) Calculate the Absorbance Ratio of the caramel colour by dividing the absorbance units at 280 nm multiplied by 20 (dilution factor) by the absorbance units at 560 nm.

PURITY TESTS

Solids content

The solids content of Caramel Colour is determined by drying a sample upon a carrier composed of pure quartz sand that passes a No. 40 but not a No. 60 sieve and has been prepared by digestion with hydrochloric acid, washed acid-free, dried and ignited. Mix 30.0 g of prepared sand accurately weighed with 1.5-2.0 g Caramel Colour accurately weighed and dry to constant weight at 60° under reduced pressure 50 mm/Hg (6.7 kPa). Record the final weight of the sand plus caramel. Calculate the % solids as follows:

$$\% \text{ solids} = \frac{(w_F - w_S)}{w_C} \text{ x } 100$$

where
w_F = final weight of sand plus caramel
w_S = weight of sand
w_C = weight of caramel initially added

Calculation on a solids basis: The contents of Total Nitrogen, Total sulfur, Ammoniacal nitrogen, sulfur dioxide, 4-MEI and THI are expressed on a solids basis. The concentration (C_I) of each impurity is determined on an "as is" basis; the concentration (C_S) on a solid basis is then calculated using the formula:

$$C_S = \frac{C_i \text{ x } 100}{\% \text{ solids}}$$

Colour Intensity

For the purpose of this specification, Colour Intensity is defined as the absorbance of a 0.1% (w/v) solution of Caramel Colour solids in water in a 1 cm cell at 610 nm.

Procedure: Transfer 100 mg of Caramel Colour into a 100 ml volumetric flask, dilute to volume with water, mix and centrifuge if the solution is cloudy. Determine the absorbance (A_{610}) of the clear solution in a 1 cm cell at 610 nm with a suitable spectrophotometer previously standardized using water as a reference. Calculate the Colour Intensity of the Caramel Colour as follows:

$$\text{Colour intensity} = \frac{A_{610} \text{ x } 100}{\% \text{ solids}}$$

Determine % solids as described under Solids content.

Calculation on an equivalent colour basis: Where additional limits for 4-MEI and THI are expressed on an equivalent colour basis the concentrations are first calculated on a solids basis as directed under "Calculations on a solids basis", and then expressed on an equivalent colour basis according to the formula:

$$\text{Equivalent colour basis} = \frac{C_S}{\text{Colour intensity}} \text{ x } 0.1$$

where C_S = concentration on a solids basis.

This gives content expressed in terms of a product having a Colour Intensity of 0.1 absorbance units.

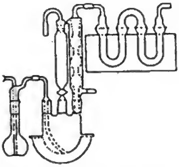
Total sulfur

In the largest available casserole that fits in an electric muffle furnace, place 1-3 g MgO or equivalent quantity of $Mg(NO_3)_2. \cdot 6H_2O$ (6.4 - 19.2 g), 1 g powdered sucrose, and 50 ml HNO_3. Add 5-10 g caramel colour. Place same quantities of reagents in another casserole for blank. Evaporate on steam bath to paste. Place casserole in cold electric muffle (25°) and gradually heat until all NO_2 fumes are driven off. Cool, dissolve and neutralize with HCl (1+2.5), adding excess of 5 ml. Filter, heat to boiling, and add 5 ml 10% $BaCl_2 \cdot 2H_2O$ solution dropwise. Evaporate to 100 ml, let stand overnight, filter, wash, ignite, and weigh the $BaSO_4$. Correct result for $BaSO_4$ obtained in blank and report as mg S/100 g. Commercial instruments that analyse for total sulfur such as, the the Leco-Combustion/Titration procedure can also be used and are recommended for sample amounts of about 200 mg.

Sulfur dioxide

Apparatus

Use a modified Monier-Williams apparatus (available from 5GA Scientific, Inc., Bloomfield, N.J., USA) for the determination of sulfurous acid, or construct the apparatus as shown in the figure. The assembly consists of a 1000-ml three-neck round-bottom distillation flask having 24/40 standard-taper ground-glass joints. A 30-cm Allihn condenser is attached in the reflux position to an outer neck of the flask, and the other end of the condenser is connected with 1/4-inch. Tygon or silicon tubing (preboiled with 1 in 20 hydrochloric acid solution and rinsed with water) to the absorption tube assembly (having 35/20 ball joints or the equivalent). Connect the centre neck of the flask with a 125-ml cylindrical separator, and attach a piece of tubing to a short U-tube inserted through a rubber stopper in the neck of the separator. Attach a curved glass inlet tube, reaching nearly to the bottom of the flask, to the other outer neck of the flask, and connect the inlet tube to a 250-ml gas-washing bottle with a piece of the tubing. The gas-washing bottle, in turn, is connected by tubing to a nitrogen cylinder.



Grind 4.5 g of pyrogallol (pyrogallic acid) with 5 ml of water in a small mortar, and transfer the slurry to the gas-washing bottle. Grind the residue again, and transfer it quantitatively to the bottle with two 5-ml portions of water. Pass nitrogen from the cylinder to the bottle to flush out air, and then add to the bottle, through a long-stem funnel, a cooled solution of 65 g of potassium hydroxide in about 85 ml of water. Place the head of the bottle in position, and bubble nitrogen through it to remove air from the headspace. Clamp off the tubing on both sides of the bottle, and connect it to the glass inlet tube of the distillation flask. The gas-washing bottle must be prepared with fresh pyrogallol solution as described on the day of use.

To each U-tube of the absorption tube assembly add the following: two pieces of 8-mm glass rod about 25 mm in length, 10 ml of 3-mm glass beads at the exit side, 10.0 ml of 3% hydrogen peroxide solution, and 1 drop of methyl red TS.

Assemble all pieces of the apparatus, and check for leaks by blowing gently into the tubing attached to the neck of the separator. While blowing, close the stopcock of the separator. Let stand for a few min; if the liquid levels in the U-tubes equalize, reseal all connections and test again. If the system is airtight proceed as directed below.

Procedure

Disperse about 25 g of the sample, accurately weighed, in 300 ml of recently boiled and cooled water, and transfer the slurry to the flask with the aid of water, using a large-bore funnel. Dilute to about 400 ml with water, and reseal the separator. Add 90 ml of 4 N hydrochloric acid to the separator, and force the acid into the flask by blowing gently into the tube in the neck of the separator. Close the stopcock of the separator.

Unclamp the tubing on both sides of the gas-washing bottle, and start the nitrogen flow at a steady stream of bubbles. Heat the distilling flask with a heating mantle to cause refluxing in approximately 20 min. When steady refluxing is reached, apply the line voltage to the mantle and reflux for 1.75 h. Turn off the water in the condenser, and continue heating until the inlet joint of the first U-tube shows condensation and slight warming. Remove the separator and turn off the heat.

When the joint at the top of the condenser cools, remove the connecting assembly and rinse it into the second U-tube, leaving the crossover tube attached to the exit joint of the first U-tube but disconnected from the entrance of the second U-tube. Rotate the crossover tube until the free end almost touches the entrance of the first U-tube. Add 1 drop of methyl red TS to the first U-tube, and titrate with 0.1 N sodium hydroxide just to a clear yellow colour, mixing with a gentle rocking motion. After titrating the first U-tube, remove the crossover tube, attach it to the second U-tube exit, and titrate similarly. Record the sum of the two titers as S, in ml.

Perform a blank determination, and record the volume of 0.1 N sodium hydroxide required as B. Calculate the percentage of sulfur dioxide in the sample by the formula

$$SO_2\,\% = \frac{(S - B) \times 0.0032 \times 100}{W}$$

where W is the weight of the sample taken, in g.

Ammonium nitrogen

Add 25 ml of 0.1 N sulfuric acid to a 500-ml receiving flask, and connect it to a distillation apparatus consisting of a Kjeldahl connecting bulb and a condenser such that the condenser delivery tube is immersed beneath the surface of the acid solution in the receiving flask. Transfer about 2 g of caramel colour, accurately weighed, into an 800-ml long-neck Kjeldahl digestion flask, and to the flask add 2 g of magnesium oxide (carbonate-free), 200 ml of water, and several boiling chips. Swirl the digestion flask to mix the contents, and quickly connect it to the distillation apparatus. Heat the digestion flask to boiling, and collect about 100 ml of distillate in the receiving flask. Wash the tip of the delivery tube with a few ml of water, collecting the washings in the receiving flask, then add 4 or 5 drops of methyl red indicator (500 mg of methyl red in 100 ml of alcohol), and titrate with 0.1 N sodium hydroxide, recording the volume, in ml, required as S. Conduct a blank determination, and record the volume, in ml, of 0.1 N sodium hdyroxide required to neutralize as B. Calculate the percentage of ammoniacal nitrogen in the sample by the formula:

$$\text{Ammoniacal nitrogen} = \frac{(B - S) \times 0.0014 \times 100}{W}$$

where W is the weight of caramel colour taken, in g.

4-Methylimidazole

NB: Information on an improved method is sought.

The following materials and reagents are required (the reagents should be ACS grade or equivalent where applicable).

Materials

Pyrex glasswool, 22 x 300 mm chromatography column with PTFE stopcock (e.g. Kimax 17800); 150 ml polypropylene beaker (e.g. Nalge 1201); 250 ml round-bottom flask (e.g., Pyrex 4320); 75 mm powder funnel; 5 cm spatula; rotary vacuum evaporator; hot plate; pan for water bath; disposable Pasteur pipets; 5 ml volumetric flask.

Reagents

Acetone; Celite 545; methylene chloride; sodium hydroxide; and tetrahydrofuran.

Procedure

After thoroughly mixing the caramel colour sample by shaking or stirring, weigh a 10.00 g aliquot into a 150 ml polypropylene beaker. Polypropylene is considered superior to glass because of its hydrophobic surface which facilitates quantitative sample transfer. A 5.0 g portion of 3.0 N NaOH is added and thoroughly mixed to ensure that the pH of the entire sample exceeds 12. A 20 g portion of Celite 545 is added to the beaker, and the contents are mixed until a semi-dry mixture is obtained. This normally requires approximately 2 to 3 min. With samples of unusually high water content, the resultant caramel colour-Celite 545 mixture may be overly wet. In such cases, a 5.00 g aliquot of caramel colour may be mixed with 2.5 g of 3.0 N NaOH and 15 g of Celite 545 and carried through the remainder of the analysis.

A plug of Pyrex glasswool is placed in the bottom of a 22 x 300 mm chromatographic column with PTFE stopcock. The caramel colour-Celite 545 mixture is placed in the column with the aid of a 75 mm powder funnel. The column contents are settled by repeatedly allowing the column to fall vertically about 10 cm to a padded surface. When properly settled, the caramel colour-Celite 545 mixture should occupy approximately the lower 250 mm of the column. Care should be exercised at this point to avoid a column bed which is either too loosely or too tightly packed. Loose packing will allow too rapid elution of the methylene chloride and possibly incomplete extraction. A too tightly packed column, e.g., the result of tamping down the column contents, can result in regions of the bed which are relatively inaccessible to the extraction solvent. This can also result in incomplete extraction.

With the stopcock open, the column is filled with methylene chloride poured from the sample beaker. When the solvent reaches the glasswool plug, the stopcock is closed and the solvent is allowed to stand in contact with the bed for 5 min. The stopcock is then opened and the column is further eluted with methylene chloride until 200 ml have been collected in a 250 ml round-bottom flask. A 1.00 ml aliquot of 2 MEI internal standard solution (50.0 mg of 2 MEI/50.0 ml of methylene chloride) is added to the collected eluate. The 2 MEI is well separated from the 4 MEI under the GLC conditions employed and has not been found in caramel colour.

The bulk of the solvent is then removed from the eluate on a rotary vacuum evaporator operated at 45-50 kPa and with the round-bottom flask maintained at 35° in a water bath. The extracted residue is transferred quantitatively to a 5 ml volumetric flask with a disposable Pasteur pipet, by rinsing the round-bottom flask several times with small (ca. 0.75 ml) portions of either tetrahydrofuran or acetone. Both solvents have been used with equal success. After mixing the contents thoroughly by several inversions of the flask, the extract is ready for GLC analysis. The extracts should be analysed as soon as possible after their preparation, because stability problems have occasionally been encountered with extracts more than 1 day old.

The GLC analysis is carried out using a gas chromatograph equipped with a hydrogen flame detector. The column is glass, 1 mm x 6 mm o.d. x 4 mm i.d., filled with 7.5% Carbowax 20M + 2% KOH on 90/100 mesh Anakrom ABS. The GLC parameters are as follows: carrier, nitrogen, 50 ml/min; hydrogen, 50 ml/min; oxygen, 80 ml/min; injection port, 200°; column isothermal, 180°; detector, 250°; sample size, 5 µl. All quantitation is done by using the internal standard technique.

2-Acetyl-4-tetrahydroxybutylimidazole (THI)

NB: Information on an improved method is sought.

THI is converted into its 2,4-dinitrophenylhydrazone (THI-DNPH). This derivative is separated from excess reagent and carbonylic contaminants by HPLC on RP-8, then determined by its absorbance at 385 nm.

Procedure

Caramel colour (200-250 mg) is weighed accurately, then dissolved in water (3 ml). The solution is transferred quantitatively to the upper part of a Combination Column. Elution with water is started, and a total of about 100 ml of water is passed through the columns.

The upper column is then disconnected. The lower column is eluted with 0.5 N HCl. The first 10.0 ml of eluate are discarded, then a volume of 35 ml is collected.

The solution is concentrated to dryness at 40° and 15 torr. The syrup residue is dissolved in carbonyl-free methanol (250 µl) and the 2,4-dinitrophenylhydrazine reagent (250 µl) is added. The reaction mixture is transferred to a septum-capped vial and stored for 5 h at room temperature.

A volume of 5 µl (but also from 1 to 25 µl) is injected onto a LiChrosorb RP-8 (10 µm) HPLC column. The mobile phase is MeOH/0.1 M H_3PO_4 50/50 (v/v). Adjustments in mobile phase composition may be needed as column characteristics vary, depending upon the manufacturer. (Use of LiChrosorb RP-8, 10 µm, 250 x 4 mm "Vertex" column manufactured by Knauer, Bad Homburg, F.R.G. is strongly recommended). At a mobile phase flow rate of 2 ml/min and column dimensions of 250 x 4.6 mm, THI-DNPH is eluted at about 6.3±0.1 min. It is detected at 385 nm and the peak height is measured. The amount is calculated from a calibration curve prepared with THI-DNPH in methanol.

Materials

- 2,4,-Dinitrophenylhydrazine hydrochloride reagent: Commercial 2,4-dinitrophenylhydrazine (5 g) is added to concentrated hydrochloric acid (10 ml) in a 100-ml erlenmeyer flask, and the latter is gently shaken until the free base (red) is converted to the hydrochloride (yellow). Ethanol (100 ml) is added and the mixture is heated on a steam bath until all the solid has dissolved. After crystallization at room temperature, the hydrochloride is filtered off, washed with ether, dried at room temperature and stored in a desiccator. On storage the hydrochloride is slowly converted to the free base. The latter can be removed by washing with dimethoxyethane. The reagent is prepared by mixing 0.5 g of 2,4-dinitrophenylhydrazine hydrochloride in 15 ml of 5% methanol in dimethoxyethane for 30 min. It should be stored in the refrigerator and be checked periodically by HPLC.
- Cation-exchange resin (strong): Dowex 50 AG x 8, H^+, 100-200 mesh.
- Cation-exchange resin (weak): Amberlite CG AG 50 I, H^+, (100-200 mesh). (Sediment two or three times prior to use).
- Methanol, carbonyl-free: Methanol is prepared after Y. Peleg and C.H. Mannheim, J. Agr. Fd. Chem, 18 (1970) 176, by treatment with Girard P reagent.
- Dimethoxyethane: If impure, dimethoxyethane is purified by distillation from 2,4-dinitrophenylhydrazine in the presence of acid and redistilled from sodium hydroxide. Immediately prior to use it is passed through a column of neutral aluminium to remove peroxides.

Instrumental

Combination Columns: Similar to the set-up described in J. Agr. Fd. Chem. 22 (1974) 110. The upper column (150 x 12.5 mm, filling height max. 9 cm, or 200 x 10 mm, filling height max. 14 cm, with capillary outlet of 1 mm i.d.) is filled with weakly acidic cation-exchanger; bed height, approx. 50-60, or 80-90 mm, respectively. The lower column (total length 175 mm, i.d. 10 mm, with capillary outlet and Teflon stopcock) is filled with strongly acidic cation-exchanger to a bed-height of 60 mm. As a solvent reservoir, a dropping funnel (100 ml) with Teflon stopcock is used. All parts are connected by standard ground-glass joints (14.5 mm).

HPLC: With the column specified above and an ultraviolet detector capable of reading at 385 nm.

Calibration: THI-DNPH is dissolved in absolute, carbonyl-free methanol (about 100 mg/l; calculated concentration of THI: 47.58 ng/µl). A portion of this solution is diluted tenfold with methanol (4.7 ng THI/µl). THI-DNPH standard solutions are stable for at least twenty weeks when stored in the refrigerator.

CARMINES

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 44th JECFA (1995) and published in FNP 52 Add 3 (1995). An ADI 0-5 mg/kg bw was established at the 26th JECFA (1982).

SYNONYMS

Cochineal carmine, Carmine, CI Natural Red 4, CI (1975) No. 75470; INS No. 120

DEFINITION

Obtained by aqueous extraction of cochineal, which consists of the dried bodies of the female insect *Dactylopius coccus* Costa; the colouring principle is a hydrated aluminium chelate of carminic acid in which aluminium and carminic acid are thought to be present in the molar ratio 1:2.

In commercial products the colouring principle is present in association with ammonium, calcium, potassium or sodium cations, singly or in combination, and these cations may also be present in excess. Products may also contain proteinaceous material derived from the source insect, and may also contain free carminate or a small excess of aluminium cations.

Chemical names

Hydrated aluminium chelate of carminic acid (7-ß-D-glucopyranosyl-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxo-anthracene-2-carboxylic acid)

C.A.S. number

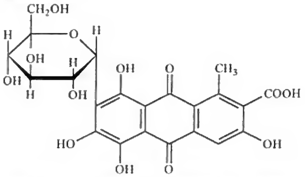
1390-65-4 (carmine)
1260-17-9 (carminic acid)

Chemical formula

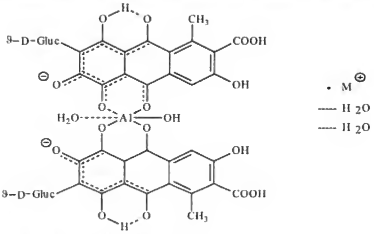
Carminic acid: $C_{22}H_{20}O_{13}$

Structural formula

Carminic acid:



Possible structural formula for the aluminium complex of carminic acid:



M^+: cation ½ Ca^{++}, Na^+, K^+, NH_4^+

Formula weight

Carminic acid: 492.39

Assay

Not less than 50% of $C_{22}H_{20}O_{13}$ on the dry basis

DESCRIPTION	Red to dark red, crumbly solid or powder
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility	The solubility of carmine preparations varies depending on the nature of the cations present. Products where the major cation is ammonium (ammonium carminate) are freely soluble in water at pH 3.0 and pH 8.5. Products where the major cation is calcium (calcium carminate) are very slightly soluble in water at pH 3.0 but freely soluble at pH 8.5.
Colour reactions	Make a solution of the sample slightly alkaline by adding 1 drop of 10% sodium hydroxide or potassium hydroxide solution. A violet colour is produced. Add a small sodium dithionite ($Na_2S_2O_4$) crystal to acid, neutral or alkaline solutions of the sample. The solutions are not decolourized. Dry a small quantity of the sample in a porcelain dish. Cool thoroughly and treat the dry residue with 1 or 2 drops of cold sulfuric acid TS. No colour change occurs. Acidify a dispersion of the sample in water with 1/3 volume of hydrochloric acid TS and shake it with amyl alcohol. Wash the amyl alcohol solution 2-4 times with an equal volume of water to remove hydrochloric acid. Dilute the amyl alcohol solution with 1-2 volumes of petroleum ether (40-60°) and shake with a few small portions of water to remove colour. Add, dropwise, 5% uranium acetate, shaking thoroughly after each addition. A characteristic emerald-green colour is produced.
PURITY	
Loss on drying (FNP5)	Not more than 20% (135°, 3h)
Total ash (FNP 5)	Not more than 12% Test 1 g of the sample as directed in the test for Ash (Total Ash)
Protein	Not more than 25% Proceed as directed under Nitrogen Determination (non-ammonia N x 6.25) (FNP 5)
Matter insoluble in dilute ammonia (FNP5)	Not more than 1% Dissolve about 0.25 g of the sample, previously dried and accurately weighed, in 2.5 ml of dilute ammonia solution (160 ml of strong ammonia TS, made up to 500 ml) and dilute to 100 ml with water: the solution is clear. Filter through a sintered glass filter (British Standard Grade No. 3). Wash with a 0.1% ammonia solution and dry to constant weight at 105°.
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, 'Instrumental methods'.
Microbiological criteria	*Salmonella:* Negative per test (FNP 5)
METHOD OF ASSAY	Weigh accurately about 100 mg of the sample, dissolve in 30 ml of boiling 2N hydrochloric acid and cool. Transfer quantitatively to a 1000-ml volumetric flask, dilute to volume with water, and mix. Determine the absorbance of the solution in a 1 cm cell at the wavelength of maximum absorbance (about 494 nm) using water as the blank. Calculate the percentage of carminic acid in the sample analysis using the formula:

$$\frac{100 \times A \times 100}{1.39 \times W}$$

where

A = absorbance of the sample solution;
W = weight, in mg, of the sample taken; and
1.39 = absorbance of a solution of carminic acid having a concentration of 100 mg per 1000 ml

If the measured absorbance of the solution is not within the range 0.650 to 0.750, prepare another sample and adjust the weight accordingly.

CELLULASE FROM *PENICILLIUM FUNICULOSUM*

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). No ADI was allocated at the 31st JECFA (1987).

SOURCES	Produced by the controlled fermentation of non-toxicogenic and non-pathogenic strains of *Penicillium funiculosum* and isolated from the growth medium.
ACTIVE PRINCIPLES	Cellulase (endo-1,4-β-glucanase) Endo-1,3(4)-β-glucanase Endo-1,4- β-xylanase
SYSTEMATIC NAMES AND NUMBERS	1,4-(1,3; 1,4)- β-D-Glucan-4-glucanohydrolase (EC 3.2.1.4) 1,3-(1,3; 1,4)- β-D-Glucan-3(4)-glucanohydrolase (EC 3.2.1.6) 1,4- β-D-xylan xylohydrolase (EC 3.2.1.8)
REACTIONS CATALYZED	Hydrolyzes 1,4-β-glucan linkages in polysaccharides such as cellulose yielding β-dextrins.
SECONDARY ENZYME ACTIVITIES	α-N-Arabinofuranosidase Cellulose 1,4- β-cellobiosidase β-glucosidase Xylan 1,4-β-xylosidase
DESCRIPTION	Typically off-white to tan amorphous powders, or liquids dispersed in food-grade carriers or diluents; soluble in water; practically insoluble in ethanol and ether.
FUNCTIONAL USES	Enzyme preparation. Used in the preparation of fruit juices, wine, beer and vegetable oils
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7).

CHARACTERISTICS

IDENTIFICATION

Cellulase activity	The sample shows cellulase activity See description under TESTS
Glucanase activity (FNP 5)	The sample shows glucanase activity
Xylanase activity	The sample shows xylanase activity See description under TESTS

TESTS

Cellulase activity

Principle

The assay is based on the ability of the enzyme to hydrolyze carboxymethyl cellulose (CMC) to reducing sugars. The reaction products are determined photometrically at 540 nm by measuring the resulting increase in reducing groups using 3,5-dinitrosalicylic acid. One cellulase unit is defined as the amount of enzyme that liberates reducing sugar at the rate of 1 μmol/min under the conditions of the assay.

Apparatus

Spectrophotometer set at 540 nm.
Water-bath set at 40.0 ± 0.1°

Reagents

1. CMC substrate solution (1.0%): Accurately weigh 0.500 g of CMC (SIGMA C5678-7 or equivalent) and sprinkle on to warm 40 ml of water in a beaker. Place

beaker on a hot-plate equipped with a magnetic stirrer, apply heat and stir vigorously. When the liquid has started to boil, cover the beaker with a watch glass, turn off the hot plate and continue stirring until the solution is cool. Quantitatively transfer the solution into a 50 ml volumetric flask, add 5 ml acetate buffer, adjust the pH to 5.0 and make up to volume.

2. 3,5-Dinitrosalicylic acid (DNS) solution: Accurately weigh 10 g of DNS into a 2000-ml beaker. Add 16 g of sodium hydroxide pellets, 300 g of potassium sodium (+)-tartrate and 500 ml of water. Place the beaker on a heater/stirrer and warm gently, whilst stirring, to dissolve. Cool to ambient temperature and transfer the contents of the beaker into a 1000-ml volumetric flask. Rinse the beaker with water, add to volumetric flask and make up to volume with water. Store the solution at ambient temperature for up to 10 weeks. It is possible that DNS reagent get overheated during the preparation making the solution quite dark. The maximum absorbance at 540 nm for a blank (without glucose standard) measured against water shall not be more than 0.050 absorbance units.

3. DNS-lactose solution: Dissolve lactose monohydrate with water to obtain 0.120 g/l solution. Mix 150 ml of DNS solution and 50 ml of Lactose solution. Use freshly prepared mixture.

4. Samples preparation: Dissolve known quantity of sample in distilled water. Make serial dilutions to get a working solution in the absorbance range of
0.150 – 0.400

5. Glucose standard solution: Accurately weigh 0.5g of anhydrous glucose and make up to volume in a 100 ml volumetric flask. Dilute the solution with water to get 5, 10 and 15 μmoles/l of glucose.

Procedure

Measurement of enzyme activity

Add 1 ml of substrate solution (pre-warmed to 40.0± 0.1° for 5 min) to an equal volume of sample solution also pre-warmed to 40.0 ± 0.1°. Mix the resulting solution thoroughly and transfer to a water-bath maintained at 40.0 ± 0.1 °. After 10 minutes (reaction step) remove the test tube from the water bath, and add 4 ml of DNS-Lactose solution and mix to stop the enzymatic reaction. Cover tubes and place in a boiling water bath for 15 min. and then cooled to room temperature with a cooling water bath. Remove insoluble substances by centrifugation (3000 rpm, 10 min). Determine the absorbance at 540 nm against water blank. Prepare a reaction blank in a similar manner but without a reaction step. Prepare a reagent blank omitting substrate and read absorbance against water.

Standard curve:

Prepare the glucose standard curve by adding 1 ml glucose standard solution (5, 10 and 15 μmoles/l) instead of CMC substrate solution in the procedure described above. Draw the standard curve in a coordinate system using glucose concentration (μmol/l) as the abscissa and absorbance as the ordinate. The standard curve is a straight line passing through the origin and linear regression can therefore be applied.

Calculate the glucose concentration in the sample from the standard curve and calculate the enzyme activity as follows.

Calculation:

Calculate the sample enzyme activity (U/g) by reading the equivalent glucose concentration on the standard curve for the sample and the reaction blank and inserting them in the following formula:

$$\text{Cellulase Activity, U / g} = \frac{(C_G - C_{RB}) \times D}{W \times 10 \times V}$$

Where

C_G : Reading from the standard curve for sample enzyme, µmol/l

C_{RB} : Reading from the standard curve for reagent blank, µmol/l

D : Dilution factor of the sample

W : Weight of sample taken, g

10 : Incubation time, min

V : Volume of sample solution taken, 1 ml

Xylanase activity

Principle

This assay is based on the enzymatic hydrolysis of sodium arabinoxylan. The resulting reducing sugar is allowed to react with 3,5-dinitrosalicylic acid and is determined photometrically at 540 nm. One xylanase unit is defined as that quantity of enzyme that liberates reducing sugar at a rate of 1 µmol /min under the conditions of the assay.

Apparatus

Spectrophotometer set at 540 nm.
Water bath set at 40.0 ± 0.1°

Reagents and solutions

1. Xylan substrate solution (1.0%): Accurately weigh 1.0 g xylan (dry base, from oat spelts; such as SIGMA X-0627), transfer to a beaker with 60 ml of 0.2 M acetate buffer (pH 4.5). Stir for 30 min and incubate at 60 ° for 1 hr with gradually stirring and check pH (4.50 ± *0.05)*. Transfer the solution into a 100 ml volumetric flask and make up to volume with water.

2. 3,5-Dinitrosalicylic acid (DNS) solution: Accurately weigh 10 g of DNS into a 2000-ml beaker. Add 16 g of sodium hydroxide pellets, 300 g of potassium sodium (+)-tartrate and 500 ml of water. Place the beaker on a heater/stirrer and warm gently, whilst stirring, to dissolve. Cool to ambient temperature and transfer the contents of the beaker into a 1000-ml volumetric flask. Rinse the beaker with water, add rinsings to the volumetric flask and make up to volume with water. Store the solution at ambient temperature for up to 10 weeks. It is possible that DNS reagent get overheated during the preparation making the solution quite dark. The maximum absorbance at 540 nm for a blank (without xylose standard) measured against water shall not be more than 0.050 absorbance units.

3. DNS-lactose solution: Dissolve lactose monohydrate with water to obtain 0.120 g/l solution. Mix 150 ml of DNS solution and 50 ml of Lactose solution. Use freshly prepared mixture.

4. Samples preparation: Dissolve known quantity of sample in distilled water. Make serial dilutions to get a working solution in the absorbance range of 0.150 – 0.400

5. Xylose standard dilutions: Accurately weigh 0.5g of anhydrous xylose with distilled water and make up to 100 ml in a volumetric flask. Dilute with water to get working standard solutions containing 250, 500 and 750 µmoles/l of xylose.

Procedure

Measurement of enzyme activity

Add 0.1 ml of sample solution to 1.9 ml of substrate solution pre-warmed to 40.0 ± 0.1° for 5 min. Mix the resulting solution thoroughly and transfer to a water-bath maintained at 40 ± 0.1°. After 10 minutes (reaction step) remove the test tube from the water bath, and add 4 ml of DNS-Lactose solution and mix to stop the enzymatic reaction. Cover tubes and place in a boiling water bath for 15 min. and then cooled to room temperature with a cooling water bath. Remove insoluble substances by a centrifuge (3000 rpm, 10 min). Determine the absorbance at 540 nm against water blank. Prepare a reagent blank in a similar manner but without a reaction step.

Standard curve:
Prepare the xylose standard curve by adding 0.1 ml xylose standard solution (250, 500 and 750 µmoles/l) instead off xylan substrate solution in the procedure described above. Draw the standard curve in a coordinate system using glucose concentration (µmol/l) as the abscissa and absorbance as the ordinate The standard curve is a straight line passing through the origin and linear regression can therefore be applied.

Calculate the xylose concentration in the sample from the standard curve and calculate the enzyme activity as follows.

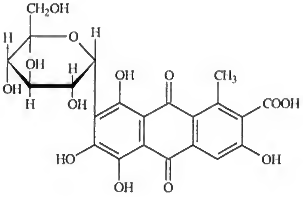
Calculation:
Calculate the sample enzyme activity (U/g) by reading the equivalent xylose concentration on the standard curve for the sample and the reaction blank and inserting them in the following formula:

$$\text{Xylanase Activity, U / g} = \frac{(C_X - C_{RB}) \text{ x } D}{W \text{ x } 10 \text{ x } V}$$

Where
C_x : Reading from the standard curve for sample enzyme, µmol/l
C_{RB}: Reading from the standard curve for reagent blank, µmol/l
D : Dilution factor of the sample
W : Weight of sample taken, g
10 : Incubation time, min
V : Volume of sample taken, 0.1 ml

COCHINEAL EXTRACT

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 51st JECFA (1998) and published in FNP 52 Add 6 (1998). No ADI was allocated at the 21st JECFA (1977).

SYNONYMS	CI Natural Red 4, CI (1975) No. 75470; INS No. 120
DEFINITION	Cochineal consists of the dried bodies of the female insect *Dactylopius coccus* Costa; Cochineal extract is the concentrated solution obtained after removing the alcohol (ethanol and/or methanol) from an aqueous, aqueous alcoholic or alcoholic extract of cochineal; the colouring principle is chiefly carminic acid; commercial products may also contain proteinaceous material derived from the source insect. In commercial products the colouring principle may also be present in association with ammonium, potassium or sodium cations, singly or in combination, and these cations may also be present in excess.
Chemical names	7-ß-D-glucopyranosyl-3,5,6,8-tetrahydroxy-1-methyl-9,10-dioxoanthracene-2-carboxylic acid
C.A.S. number	1343-78-8 (cochineal) 1260-17-9 (carminic acid)
Chemical formula	$C_{22}H_{20}O_{13}$ (Carminic acid)
Structural formula	Carminic acid:  CH₂OH H O H OH H OH H OH OH O CH₃ COOH HO OH OH O
Formula weight	Carminic acid: 492.39
Assay	Not less than 2.0% $C_{22}H_{20}O_{13}$
DESCRIPTION	Dark red liquid
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Freely soluble in water
Colour reactions	Make a solution of the sample slightly alkaline by adding 1 drop of 10% sodium hydroxide or potassium hydroxide solution. A violet colour is produced. Add a small sodium dithionite ($Na_2S_2O_4$) crystal to acid, neutral or alkaline solutions of the sample. The solutions are not decolourized.

Dry a small quantity of the sample in a porcelain dish. Cool thoroughly and treat the dry residue with 1 or 2 drops of cold sulfuric acid TS. No colour change occurs.

Acidify a dispersion of the sample in water with 1/3 volume of hydrochloric acid TS and shake it with amyl alcohol. Wash the amyl alcohol solution 2-4 times with an equal volume of water to remove hydrochloric acid. Dilute the amyl alcohol solution with 1-2 volumes of petroleum ether (40-60°) and shake with a few small portions of water to remove colour. Add, dropwise, 5% uranium acetate, shaking thoroughly after each addition. A characteristic emerald-green colour is produced.

PURITY

Protein	Not more than 2.2% Proceed as directed under Nitrogen Determination (non-ammonia N x 6.25) (FNP 5)
Ethanol (FNP 5)	Not more than 150 mg/kg Proceed as directed under Residual solvent
Methanol (FNP 5)	Not more than 150 mg/kg Proceed as directed under Residual solvent
Microbiological criteria	*Salmonella:* Negative per test (FNP 5)
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, 'Instrumental methods'

METHOD OF ASSAY

Weigh accurately about 1 g of the sample, dissolve in 30 ml of boiling 2N hydrochloric acid, and cool. Transfer quantitatively to a 1000 ml volumetric flask, dilute to volume with water, and mix. Determine the absorbance of the solution in a 1 cm cell at the wavelength of maximun absorbance (about 494 nm) using water as the blank. Calculate the percentage of carminic acid in the sample using the formula:

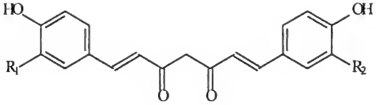
$$\frac{100 \times A \times 100}{1.39 \times W}$$

where
A = absorbance of the sample solution;
W = weight, in mg, of the sample taken; and
1.39 = absorbance of a solution of carminic acid having a concentration of 100 mg per 1000 ml

If the measured absorbance is not within the range 0.650 to 0.750, prepare another sample and adjust the weight accordingly.

CURCUMIN

Prepared at the 55th JECFA (2000) and published in FNP Add 8 (2000), superseding tentative specifications prepared at the 51st JECFA (1998) and published in FNP 52 Add 6 (1998). A temporary ADI of 0-1 mg/kg bw was established at the 44th JECFA (1995) and extended at the 51st JECFA (1998).

SYNONYMS	Curcumin, Turmeric yellow, Diferuloylmethane, Kurkum, CI Natural Yellow 3, CI (1975) 75300; INS No. 100(i)
DEFINITION	The main colouring principles are curcumin (1,7-bis-(4-hydroxy-3-methoxy-phenyl)-hepta-1,6-diene-3,5-dione and its desmethoxy- and bis-desmethoxy-derivatives in varying proportions. Curcumin is obtained by solvent extraction of turmeric i.e., the ground rhizomes of *Curcuma domestica (Curcuma longa L).* In order to obtain a concentrated curcumin powder, the extract is purified by crystallization; minor amounts of oils and resins naturally occurring in turmeric may be present. Only the following solvents may be used in the extraction: acetone, methanol, ethanol, isopropanol, hexane.
Chemical names	Principal colouring components: I. 1,7-Bis-(4-hydroxy-3-methoxyphenyl)-hepta-1,6-diene-3,5-dione II. 1-(4-Hydroxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-hepta-1,6-diene-3,5-dione III. 1,7-Bis-(4-hydroxyphenyl)-hepta-1,6-diene-3,5-dione
C.A.S. number	458-37-7
Chemical formula	I. $C_{21}H_{20}O_6$ II. $C_{20}H_{18}O_5$ III. $C_{19}H_{16}O_4$
Structural formula	 I. $R_1 = R_2 = -OCH_3$ II. $R_1 = -OCH_3, R_2 = H$ III. $R_1 = R_2 = H$
Formula weight	I. 368.39 II. 338.39 III. 308.39
Assay	Not less than 90% total colouring matters
DESCRIPTION	Orange-yellow crystalline powder
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water and in diethyl ether; soluble in ethanol and in glacial acetic acid

Melting range (FNP 5)

179 - 182°

Colour reactions

A solution of the sample in ethanol is characterized by pure yellow colour and light green fluorescence; if this ethanol extract is added to concentrated sulfuric acid, a deep crimson colour is produced.

Treat an aqueous or dilute ethanolic solution of the sample with hydrochloric acid until a slightly orange colour begins to appear. Divide mixture into 2 parts and add some boric acid powder or crystals to one portion. Marked reddening will be quickly apparent, best seen by comparison with portion to which the boric acid has not been added. The test may also be made by dipping pieces of filter paper in ethanolic solution of colouring matter, drying at 100°, and then moistening with a weak solution of boric acid to which a few drops of hydrochloric acid have been added. On drying, a cherry-red colour will develop.

Chromatography

Spot 5 µl of test solution (0.01 g of sample in 1 ml of 95% ethanol) on a TLC (Microcrystalline cellulose, 0.1 mm) plate. Develop the plate in a chamber containing a mixture of 3-methyl-1-butanol/ethanol/ water/ammonia (4:4:2:1) as solvent and allow the solvent front to ascend 10-15 cm. Examine under daylight and under UV-light and observe:
- Three yellow spots with R_f between 0.2 and 0.4 under daylight and UV-light
- Spots with R_f about 0.6 and 0.8 under UV-light

All spots show distinct yellow fluorescence under UV-light.

PURITY

Residual solvents (FNP 5)

Acetone: Not more than 30 mg/kg
Methanol: Not more than 50 mg/kg
Ethanol: Not more than 50 mg/kg
Isopropanol: Not more than 50 mg/kg
Hexane: Not more than 25 mg/kg

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described on FNP 5, "Instrumental methods".

METHOD OF ASSAY

Accurately weigh about 0.08 g of the sample. Transfer to a 200-ml volumetric flask with ethanol and swirl to dissolve. Make up to volume with ethanol and mix. Prepare a 100-times diluted solution with ethanol.

Determine the absorbance (A) at 425 nm in a 1-cm cell. Calculate the total colouring matters content of the sample using the following equation.

% Total Colouring matters:

$$\frac{A \times 20 \times 1000}{W \times 1607}$$

where
A = absorbance of sample
W = weight of sample (g)

The determination must be performed without delay, because the colour fades.

DIATOMACEOUS EARTH

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 21st JECFA (1977) and published in NMRS 57 (1977) and in FNP 52 (1992).

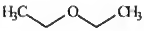
SYNONYMS	Diatomaceous silica, Diatomite
DEFINITION	Consists of the processed siliceous skeletons of diatoms; produced as a dried, natural powder, as a calcined powder or as a flux-calcined powder.
C.A.S. number	Natural and calcined powder 61790-53-2 Flux-calcined 68855-54-9
DESCRIPTION	Dried, natural powder: off-white to light grey. Calcined powder: pink to light brown or light yellow to light orange. Flux-calcined powder: white to pink or light brown.
FUNCTIONAL USES	Filtering aid
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, in acids (except hydrofluoric), and in dilute alkalis
Microscopy	When examined with 100x to 200x microscope, typical diatom shapes are observed
pH	Boil 10 g of sample with 100 ml of water for 1 h and filter through a fine-porosity sintered-glass filter or a suitable filter paper. Dilute filtrate to 100 ml. Natural and calcined powders, pH range: 5 to 10. Flux-calcined powders, pH range: 8 to 11.
Volatilization	Place 0.2 g of the sample in a platinum crucible, and add 5 ml of hydrofluoric acid. The sample is dissolved. When the solution is heated (Caution: Use draft oven), almost all of it volatilizes.
PURITY	
Loss on drying (FNP 5)	Natural powder: Not more than 10% (105°, 2 h) Calcined and flux-calcined powder: Not more than 3% (105°, 2 h)
Loss on ignition (FNP 5)	Natural powder: Not more than 7% on the dry basis Calcined and flux-calcined powder: Not more than 2% on the dry basis.
Hydrofluoric acid-insoluble substances	Not more than 25% Weigh accurately about 0.2 g of the dried sample in a platinum crucible previously ignited, cooled, and weighed. Add 5 ml of hydrofluoric acid and 2 drops of sulfuric acid (1 in 2), and evaporate gently to approximate dryness on a water bath. Heat at 550° for 1 h, then raise the temperature gradually until it reaches 1000° to 1200°, and keep the temperature for 30 min. The residue does not exceed 50 mg.
Water-soluble substances	Not more than 0.5% To 10 g of the dried sample, add 100 ml of water, and boil for 2 h, supplementing water with occasional shaking. Cool, then filter with suction using a filter paper for quantitative analysis. Repeat the filtration using the same filter paper to obtain a clear solution. Wash the residue on filter paper with a small amount of water. Combine washings to filtrate, evaporate the solution to dryness and dry further the residue at 105° for 2 h. The weight of the residue is not more than 50 mg.

Hydrochloric acid-soluble substances	Not more than 2.5% To 2.0 g of the dried sample, add 50 ml of dilute hydrochloric acid TS, and heat at 50° for 15 min with shaking. Cool and filter, wash filter residue with a small amount of dilute hydrochloric acid TS. Combine washings to filtrate, add 5 ml of dilute sulfuric acid TS, evaporate to dryness, and ignite at 450-550° to constant weight. The weight of the residue is not more than 50 mg.
Arsenic (FNP 5)	Not more than 10 mg/kg Transfer 2.5 g of the sample into a 250-ml beaker, add 50 ml of hydrochloric acid, cover with a watch glass, and heat at 70° for 15 min with shaking. Cool, and decant through a filter paper into a 100-ml volumetric flask. Wash the slurry with three 10-ml portions of hot water and the filter paper with 15 ml of hot water. Dilute to volume with water and mix. A 10-ml portion of this solution meets the requirements of the Limit Test (Method II).
Lead	Not more than 10 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP5, "Instrumental Methods".

DIETHYL ETHER

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 37th JECFA (1990) and published in FNP 52 (1992). No ADI was allocated at the 37th JECFA (1990).

Warning: Determination to be made only after ensuring that the sample complies with the test for peroxides. It is dangerous to distil or evaporate Diethylether which does not comply with the Test for peroxides (FNP 5).

SYNONYMS	Ether, Ethyl ether
DEFINITION	Diethyl ether normally contains appropriate stabilizers such as pyrogallol or BHT. Manufacturers should indicate on the label the specific stabilizer(s) used and the amount added. Typical levels are in the range of 3-7 mg/l.
Chemical names	Diethyl ether, diethyl oxide, 1,1'-oxybisethane
C.A.S. number	60-29-7
Chemical formula	$C_4H_{10}O$
Structural formula	
Formula weight	74.12
DESCRIPTION	Colourless, clear, very mobile liquid, with a characteristic odour; very volatile and flammable.
FUNCTIONAL USES	Extraction solvent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water; miscible with ethanol
Specific gravity (FNP 5)	0.714 - 0.716
PURITY	
Distillation range (FNP 5)	34 - 35° (see warning above)
Non-volatile residue (FNP 5)	Not more than 2 mg/100 ml (see warning above)
Water (FNP 5)	Not more than 0.2% (Karl Fischer Method)
Acidity	To 20 ml of 95% ethanol in a 50-ml stoppered measuring cylinder, add 0.5 ml of phenolphthalein TS and just sufficient 0.02 N sodium hydroxide to produce a pink colour which persists after gentle shaking for 30 sec. Add a further 0.3 ml of 0.02 N sodium hydroxide and 25 ml of the sample, stopper the cylinder, mix and shake gently for 30 sec. The pink colour is not discharged.
Aldehydes and ketones	Place 2 ml of Nessler's TS in a stoppered tube of about 12-ml capacity and about 1.5-cm diameter and fill the tube with the sample. Insert the stopper, shake vigorously for 10 sec, and allow to stand in the dark for 5 min. If no colour or turbidity is produced at this stage, the sample is considered to have complied with the test. If colour or turbidity is produced, after ensuring that the sample complies with the test for peroxides distil a further quantity of the sample in a fractionating column and repeat the test on the distillate. No colour or turbidity is produced.

Peroxides	Passes test The colour produced by iodine liberated by the action of organic peroxides on potassium iodide is compared with that of a standard iodine solution. Place 8 ml of freshly prepared 10 % potassium iodide solution in a stoppered tube of 12-ml capacity and about 1.5 cm diameter. Fill the tube to the brim with the sample, place the stopper in position so that no air bubble is enclosed, shake vigorously, and allow to stand in the dark for 30 min. The yellow colour produced, if any, is no darker than that of 0.5 ml of 0.001 N iodine diluted with 8 ml of the potassium iodide solution.
Lead	Not more than 2 mg/kg. Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods."

β-GLUCANASE FROM *TRICHODERMA HARZIANUM*

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 39th JECFA (1992) and published in FNP 52 Add 1 (1992). An ADI "Not specified" was established at the 39th JECFA (1992).

SOURCES	Produced by the controlled fermentation of non-pathogenic and non-toxicogenic strains of *Trichoderma harzianum* (classification by Rifai M.A., Mycological Papers, No. 116, pages 1-56, 1969) and isolated from the growth medium.
ACTIVE PRINCIPLES	1) Endo-1,3-β-glucanase (synonym: laminarinase) 2) Exo-1,3-β-glucanase
SYSTEMATIC NAMES AND NUMBERS	1. 1,3-(1,3; 1,4)-β-D-glucan 3(4) glucanohydrolase (EC 3.2.1.6; C.A.S. No. 62213-14-3) 2. Glucan 1,3-β-glucosidase (EC 3.2.1.58; C.A.S. No. 9073-49-8)
REACTIONS CATALYZED	Hydrolyzes β-1,3 or β-1,4 linkages in 1,3 (1,4)-β-D-glucans yielding glucose.
SECONDARY ENZYME ACTIVITIES	Hemicellulase Cellulase (1,4-[1,3;1,4]-β-D-Glucan 4-glucano-hydrolase); (EC 3.2.1.4; C.A.S. No. 9012-54-8) Pectinase (Poly (1,4-α-D-galacturonide) glycanohydrolase); (EC 3.2.1.15; C.A.S. No. 9032-75-1)
DESCRIPTION	Typically off-white to tan amorphous powders or tan to dark-brown liquids. These products are concentrated and standardised with food-grade diluents or carriers such as maltodextrin, starch or glucose to obtain commercial preparations. Soluble in water and practically insoluble in ethanol and ether.
FUNCTIONAL USES	Enzyme preparation Used in the preparation of fruit juices, wine, beer and vegetable oils
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7).

CHARACTERISTICS

IDENTIFICATION

β-Glucanase activity (FNP 5)	The sample shows β-glucanase activity

GUAIAC RESIN

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 17th JECFA (1973) and published in FNP 4 (1978) and in FNP 52 (1992). An ADI of 0-2.5 mg/kg bw was established at the 17th JECFA (1973).

SYNONYMS	Guaiac gum, Gum guaiac, Gum guaiacum, Guaiacum; INS No. 314
DEFINITION	The resin from the wood of *Guajacum officinale* L., or of *Guajacum sanctum* L., (Fam. *Zygophyllaceae*), consisting of approximately 70% alpha- and beta-guaiaconic acids, 10% guaiaretic acid, and 15% guaiac ß-resin and small quantities of guaiac yellow, vanillin, etc.
DESCRIPTION	Irregular lumps enclosing fragments of vegetable tissues; or large, nearly homogeneous masses and occasionally more or less rounded or ovoid tears; externally, it is brownish black to dusky brown, acquiring a greenish colour on long exposure, the fractured surface having a glassy lustre, the thin pieces being transparent and varying in colour from brown to yellowish orange; the powder is moderate yellow brown, becoming olive brown on exposure to air. It has a mild balsamic odour.
FUNCTIONAL USES	Antioxidant
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water; soluble in fats; dissolves readily but incompletely in ethanol, ether, and solutions of alkalis
Melting range (FNP 5)	85 - 90°
Colour reactions	Add 1 drop of ferric chloride TS to 5 ml of an ethanolic solution of the sample (1 in 100). A blue colour is produced which gradually changes to green, finally becoming greenish yellow. A mixture of 5 ml of an ethanolic solution of the sample (1 in 100) and 5 ml of water becomes blue upon shaking with 20 mg of lead peroxide. Filter the solution, and boil a portion of the filtrate. The colour disappears but may be restored by the addition of lead peroxide and shaking. Add a few drops of diluted hydrochloric acid TS to a second portion of the filtrate. The colour is immediately discharged.
PURITY	
Total ash (FNP 5)	Not more than 5%
Acid-insoluble ash (FNP 5)	Not more than 2%
Ethanol-insoluble residue	Not more than 15% Place 2 g of the sample, finely powdered and accurately weighed, in a dry, tared extraction thimble, and extract it with ethanol in a suitable continuous extraction apparatus for 3 h or until completely extracted. Dry the insoluble residue in a thimble for 4 h at 105° and weigh. The weight of the residue shall not exceed 300 mg.
Rosin	A 10% solution of the sample in petroleum ether is colourless and when shaken with an equal quantity of a fresh solution of cupric acetate 0.5% is not more green than a similar solution of cupric acetate in petroleum ether.
Lead	Not more than 2 mg/kg. Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods."

HEMICELLULASE FROM *ASPERGILLUS NIGER*, VAR

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Not specified" was established at the 35st JECFA (1989).

SOURCES	Produced by the controlled fermentation of non-pathogenic and non-toxicogenic strains of *Aspergillus niger* and isolated from the growth medium.
ACTIVE PRINCIPLES	1) Endo-1,4-β-xylanase 2) Xylan 1,4-β-xylosidase 3) α-L-Arabinofuranosidase 4) Cellulase 5) Galactomannanase
SYSTEMATIC NAMES AND NUMBERS	1) 1,4-β-D-Xylan xylanohydrolase (EC 3.2.1.8; C.A.S. No. 9025-57-4) 2) 1,4-β-D-Xylan xylohydrolase (EC 3.2.1.37; C.A.S. No. 9025-53-0) 3) α-L-Arabinofuranoside arabino-furanohydrolase (EC 3.2.1.55; C.A.S. No. 9067-74-7) 4) 1,4-[1,3; 1,4]-β-D-Glucan 4-glucano-hydrolase (EC 3.2.1.4; C.A.S. No. 9012-54-8) 5) 1,4-β-D-galactan-4-mannano-hydrolase (C.A.S. No. 50812-17-4)
SECONDARY ENZYME ACTIVITIES	1) Glucoamylase (1,4-α-D-Glucan glucohydrase; EC 3.2.1.3; C.A.S. No. 9032-08-0) 2) Maltase (α-D-Glucosidase glucohydrolase; EC 3.2.1.20; C.A.S. No. 9001-42-7) 3) Lactase (β-galactosidase, β-D-Galactoside galactohydrolase, EC 3.2.1.23, C.A.S. No. 9031-11-2) 4) Invertase (Saccharase, β-Fructofuranosidase, β-D-Fructofuranoside fructohydrolase; EC 3.2.1.26)
REACTIONS CATALYZED	Hydrolyzes the linkages between the various sugar groups of the polysaccharide chains.
DESCRIPTION	Typically off-white to tan amorphous powders or tan to dark-brown liquids. The unformulated product is usually diluted and standardised with food grade lactose, maize starch or maltodextrin powders to obtain commercial preparations. Soluble in water and practically insoluble in ethanol and ether
FUNCTIONAL USES	Enzyme preparation Used in the manufacture of instant coffee and bread making process
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7).
CHARACTERISTICS	
IDENTIFICATION	
Cellulase activity	The sample shows cellulase activity See description under TESTS
Galactomannanase activity	The sample shows galactomannanase activity See description under TESTS
Xylanase activity	The sample shows xylanase activity See description under TESTS

Cellulase activity

Principle

The assay is based on the ability of the enzyme to hydrolyze carboxymethyl cellulose (CMC) to reducing sugars. The reaction products are determined photometrically at 540 nm by measuring the resulting increase in reducing groups using 3,5-dinitrosalicylic acid. One cellulase unit is defined as the amount of enzyme that liberates reducing sugar at the rate of 1 µmol/min under the conditions of the assay.

Apparatus

Spectrophotometer set at 540 nm.
Water-bath set at 40.0 ± 0.1°

Reagents

1. CMC substrate solution (1.0%): Accurately weigh 0.500 g of CMC (SIGMA C5678-7 or equivalent) and sprinkle on to warm 40 ml of water in a beaker. Place beaker on a hot-plate equipped with a magnetic stirrer, apply heat and stir vigorously. When the liquid has started to boil, cover the beaker with a watch glass, turn off the hot plate and continue stirring until the solution is cool. Quantitatively transfer the solution into a 50 ml volumetric flask, add 5 ml acetate buffer, adjust the pH to 5.0 and make up to volume.

2. 3,5-Dinitrosalicylic acid (DNS) solution: Accurately weigh 10 g of DNS into a 2000-ml beaker. Add 16 g of sodium hydroxide pellets, 300 g of potassium sodium (+)-tartrate and 500 ml of water. Place the beaker on a heater/stirrer and warm gently, whilst stirring, to dissolve. Cool to ambient temperature and transfer the contents of the beaker into a 1000-ml volumetric flask. Rinse the beaker with water, add to volumetric flask and make up to volume with water. Store the solution at ambient temperature for up to 10 weeks. It is possible that DNS reagent get overheated during the preparation making the solution quite dark. The maximum absorbance at 540 nm for a blank (without glucose standard) measured against water shall not be more than 0.050 absorbance units.

3. DNS-lactose solution: Dissolve lactose monohydrate with water to obtain 0.120 g/l solution. Mix 150 ml of DNS solution and 50 ml of Lactose solution. Use freshly prepared mixture.

4. Samples preparation: Dissolve known quantity of sample in distilled water. Make serial dilutions to get a working solution in the absorbance range of 0.150 – 0.400

5. Glucose standard solution: Accurately weigh 0.5g of anhydrous glucose and make up to volume in a 100 ml volumetric flask. Dilute the solution with water to get 5, 10 and 15 µmoles/l of glucose.

Procedure

Measurement of enzyme activity

Add 1 ml of substrate solution (pre-warmed to 40.0± 0.1° for 5 min) to an equal volume of sample solution also pre-warmed to 40.0 ± 0.1°. Mix the resulting solution thoroughly and transfer to a water-bath maintained at 40.0 ± 0.1 °. After 10 minutes (reaction step) remove the test tube from the water bath, and add 4 ml of DNS-Lactose solution and mix to stop the enzymatic reaction. Cover tubes and place in a boiling water bath for 15 min. and then cooled to room temperature with a cooling water bath. Remove insoluble substances by centrifugation (3000 rpm, 10 min). Determine the absorbance at 540 nm against water blank. Prepare a reaction blank in a similar manner but without a reaction step. Prepare a reagent blank omitting substrate and read absorbance against water.

Standard curve:

Prepare the glucose standard curve by adding 1 ml glucose standard solution (5, 10 and 15 µmoles/l) instead of CMC substrate solution in the procedure described above. Draw the standard curve in a coordinate system using glucose concentration (µmol/l) as the abscissa and absorbance as the ordinate. The standard curve is a straight line passing through the origin and linear regression can therefore be applied.

Calculate the glucose concentration in the sample from the standard curve and calculate the enzyme activity as follows.

Calculation:
Calculate the sample enzyme activity (U/g) by reading the equivalent glucose concentration on the standard curve for the sample and the reaction blank and inserting them in the following formula:

$$\text{Cellulase Activity, U / g} = \frac{(C_G - C_{RB}) \times D}{W \times 10 \times V}$$

Where

C_G : Reading from the standard curve for sample enzyme, µmol/l
C_{RB} : Reading from the standard curve for reagent blank, µmol/l
D : Dilution factor of the sample
W : Weight of sample taken, g
10 : Incubation time, min
V : Volume of sample solution taken, 1 ml

Galactomannanase activity

Principle
This assay method is based on the enzymatic hydrolysis of galactomannan. The velocity of the decrease of the viscosity of the substrate under the enzymatic action is measured in a capillary viscometer. One unit of galactomannanase activity (GMA) is defined as that quantity of enzyme that decreases to half the initial viscosity per minute of substrate under the conditions of the assay.

Apparatus
Capillary viscometer such as Cannon-Fenske viscometer, Type #200.
Two digital watches, calibrated in 1/10 sec.
Water-bath set at 40.0 ± 0.1 °

Reagents and solutions
1. Substrate solution: Weigh 0.73 g dry base (loss on drying value: 1g, 105°, 3 hr) of substrate Locust Bean Gum (such as SIGMA G-0735) in 500 ml beaker. Add about 400 ml of water and stir gently by a magnetic stirrer for 10 min and heat with boiling water for more than 3 min. Quantitatively transfer the solution to 500 ml volumetric flask and fill with water and then filter this solution before use.

2. Acetate buffer pH 4.5: Add 30 g of glacial acetic acid in about 800 ml of water. Adjust pH 4.5 ± 0.02 with 1N sodium hydroxide by pH meter. Quantitatively transfer the solution to 1000 ml volumetric flask, dilute to volume with water, and mix.
3. Sample solution: Dissolve in water to obtain about 0.015-0.040 U/ml enzyme activities that allows the end point of the reactions to be between 4 to 5min.

4. Enzyme standard solutions: Dilute with water Galactomannanase standard (~50,000 U/g, such as Shin Nihon Chemical Co., Ltd) to contain 0.03 U/ml.

Procedure
Allow the temperature of the viscometer to reach equilibrium with the bath thermostatically controlled at 40.0 ± 0.1 ° at least 5 minutes. Place in the bath test tubes containing 10 ml of the substrate solution and 1 ml of buffer, mix and allow it to reach equilibrium with the temperature (~5 min). At zero time measured on watch no. 1, add 1 ml of the sample or the enzyme standard solution to the test tube, mix and pour the quantity needed for the measurements into the bulb of the viscometer. Wait at least two minutes and then suck the reactive mixture into the upper measuring bulb and allow it to flow out; as soon as the meniscus of the liquid becomes tangent to the upper mark, start stop-watch No. 2 and simultaneously record

watch No. 1 (time t_1); as soon as the meniscus becomes tangent to the lower mark, stop-watch No. 2 (efflux time t_2).

Calculate the reaction time (R) as follows:
The enzyme reaction time, which the efflux of the reaction mixture has been measured, is defined as a half point from the beginning time to the end time of the efflux measurement.

$$R = t_1 + \frac{t_2}{2}$$

Repeat at different reaction times (such as 4, 6, 8 minutes) and calculate the reaction time in the same way described above.

Efflux time of the substrate blank solution
Mix 10 ml of substrate solution, 1 ml of buffer and 1 ml of water into a test tube and equilibrate at 40.0 ± 0.1 °C for about 5 min. Measure the efflux time of the substrate blank solution in the same way described above. Repeat 3 times each measurement of the efflux time, and average them (t_{2sb}).

Efflux time of the water blank
Pipet 12 ml of water in to a test tube and equilibrate at 40.0 ± 0.1°C for about 5 min. Measure the efflux time of water in the same way described above. Repeat 3 times each measurement of the efflux time, and average them (t_{2w}).

Calculation
Calculate the efflux time when the substrate blank viscosity is reduced to half of the initial viscosity value ($t_{1/2}$) as follows:

$$t_{1/2} = \frac{t_{2sb} + t_{2w}}{2}$$

Plot the efflux time (t_2) as the ordinate against the reaction time (R) as the abscissa and draw the curve. For the sample and for the standard read the end point of the reaction time (R) corresponding to 1/2 efflux time of the substrate blank ($t_{1/2}$) from the curve.

Galactomannanase activity units of the unknown sample are calculated in relation with a known standard.

$$\text{Galactomannanase, U/g} = \text{St} \times \frac{\text{Rs} \times \text{Cs}}{\text{Rx} \times \text{Cx}}$$

St: galactomannanase activity of the enzyme standard (50000 U/g)
Rs: the reaction time of the enzyme standard solution at the $t_{1/2}$ (sec)
Cs: concentration of the enzyme standard solution (g/ml)
Rx: the reaction time of sample solution at the $t_{1/2}$ (sec)
Cx: concentration of sample solution (g/ml)

Xylanase activity

Principle
This assay is based on the enzymatic hydrolysis of sodium arabinoxylan. The resulting reducing sugar is allowed to react with 3,5-dinitrosalicylic acid and is determined photometrically at 540 nm. One xylanase unit is defined as that quantity of enzyme that liberates reducing sugar at a rate of 1 µmol /min under the conditions of the assay.

Apparatus
Spectrophotometer set at 540 nm.
Water bath set at 40.0 ± 0.1°

Reagents and solutions

1. Xylan substrate solution (1.0%): Accurately weigh 1.0 g xylan (dry base, from oat spelts; such as SIGMA X-0627), transfer to a beaker with 60 ml of 0.2 M acetate buffer (pH 4.5). Stir for 30 min and incubate at 60 ° for 1 hr with gradually stirring and check pH (4.50 ± *0.05)*. Transfer the solution into a 100 ml volumetric flask and make up to volume with water.

2. 3,5-Dinitrosalicylic acid (DNS) solution: Accurately weigh 10 g of DNS into a 2000-ml beaker. Add 16 g of sodium hydroxide pellets, 300 g of potassium sodium (+)-tartrate and 500 ml of water. Place the beaker on a heater/stirrer and warm gently, whilst stirring, to dissolve. Cool to ambient temperature and transfer the contents of the beaker into a 1000-ml volumetric flask. Rinse the beaker with water, add rinsings to the volumetric flask and make up to volume with water. Store the solution at ambient temperature for up to 10 weeks. It is possible that DNS reagent get overheated during the preparation making the solution quite dark. The maximum absorbance at 540 nm for a blank (without xylose standard) measured against water shall not be more than 0.050 absorbance units.

3. DNS-lactose solution: Dissolve lactose monohydrate with water to obtain 0.120 g/l solution. Mix 150 ml of DNS solution and 50 ml of Lactose solution. Use freshly prepared mixture.

4. Samples preparation: Dissolve known quantity of sample in distilled water. Make serial dilutions to get a working solution in the absorbance range of 0.150 – 0.400

5. Xylose standard dilutions: Accurately weigh 0.5g of anhydrous xylose with distilled water and make up to 100 ml in a volumetric flask. Dilute with water to get working standard solutions containing 250, 500 and 750 µmoles/l of xylose.

Procedure

Measurement of enzyme activity

Add 0.1 ml of sample solution to 1.9 ml of substrate solution pre-warmed to 40.0 ± 0.1° for 5 min. Mix the resulting solution thoroughly and transfer to a water-bath maintained at 40 ± 0.1°. After 10 minutes (reaction step) remove the test tube from the water bath, and add 4 ml of DNS-Lactose solution and mix to stop the enzymatic reaction. Cover tubes and place in a boiling water bath for 15 min. and then cooled to room temperature with a cooling water bath. Remove insoluble substances by a centrifuge (3000 rpm, 10 min). Determine the absorbance at 540 nm against water blank. Prepare a reagent blank in a similar manner but without a reaction step.

Standard curve:

Prepare the xylose standard curve by adding 0.1 ml xylose standard solution (250, 500 and 750 µmoles/l) instead off xylan substrate solution in the procedure described above. Draw the standard curve in a coordinate system using glucose concentration (µmol/l) as the abscissa and absorbance as the ordinate The standard curve is a straight line passing through the origin and linear regression can therefore be applied.

Calculate the xylose concentration in the sample from the standard curve and calculate the enzyme activity as follows.

Calculation:

Calculate the sample enzyme activity by reading the equivalent xylose concentration on the standard curve for the sample and the reaction blank and inserting them in the following formula:

$$\text{Xylanase Activity, U/g} = \frac{(C_x - C_{RB}) \text{ x } D}{W \text{ x } 10 \text{ x } V}$$

Where

C_x : Reading from the standard curve for sample enzyme, µmol/l
C_{RB}: Reading from the standard curve for reagent blank, µmol/l
D : Dilution factor of the sample
W : Weight of sample taken, g
10 : Incubation time, min
V : Volume of sample taken, 0.1ml

MICROCRYSTALLINE CELLULOSE

Prepared at the 55th JECFA (2000) and published in FNP52 Add 8 (2000), superseding specifications prepared at the 51st JECFA (1998) and published in FNP 52 Add 6 (1998). An ADI "Not specified" was established at the 49th JECFA (1998).

SYNONYMS	Cellulose gel; INS No. 460
DEFINITION	Purified, partially depolymerized cellulose prepared by treating alpha-cellulose, obtained as a pulp from fibrous plant material, with mineral acids. The degree of polymerization is typically less than 400. Not more than 10% of the particles have a diameter below 5 µm.
Chemical names	Cellulose
C.A.S. number	9004-34-6
Chemical formula	$(C_6H_{10}O_5)_n$
Assay	Not less than 97% of carbohydrate calculated as cellulose on the dry basis.
DESCRIPTION	Fine, white or almost white, odourless, free flowing crystalline powder.
FUNCTIONAL USES	Emulsifier, stabilizer, anticaking agent, dispersing agent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, ethanol, ether and dilute mineral acids. Slightly soluble in sodium hydroxide solution
Infrared absorption	The infrared absorption spectrum of a potassium bromide dispersion of the sample corresponds to the infrared spectrum below.
Suspensoid	Mix 30 g of the sample with 270 ml of water in a high-speed (18,000 rpm) blender for 5 min. Transfer 100 ml of the mixture to a 100-ml graduated cylinder, and allow to stand for 3 h. A white, opaque, bubble-free dispersion that forms a supernatant, is obtained.
PURITY	
Loss on drying (FNP 5)	Not more than 7.0% (105 °, 3 h)
pH (FNP 5)	5.0 - 7.5 Shake 5 g of the sample with 40 ml of water for 20 min and centrifuge. Determine the pH of the supernatant.
Sulfated ash (FNP 5)	Not more than 0.05% Test 10 g of the sample (Method I)
Water soluble Substances	Not more than 0.24%. Shake 5 g of the sample with approximately 80 ml of water for 10 min, filter through Whatman No. 42 or equivalent filter paper into a tared beaker, wash residue with 20 ml of water and evaporate to dryness on a steam bath. Dry at 105° for 1 h., cool, weigh and calculate as percentage.
Starch	Not detectable To 20 ml of the dispersion obtained in the identification test for starch, add a few drops of iodine TS, and mix. No purplish to blue or blue colour should be obtained.

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

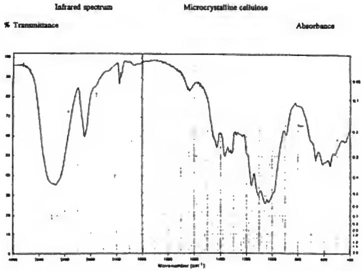
METHOD OF ASSAY

Transfer about 125 mg of the sample, accurately weighed, to a 300 ml Erlenmeyer flask, using about 25 ml of water. Add 50.0 ml of 0.5N potassium dichromate and mix. Carefully add 100 ml of sulfuric acid and heat to boiling. Remove from heat, allow to stand at room temperature for 15 min and cool in a water bath. Transfer the contents into a 250 ml volumetric flask, rinse flask with distilled water, add rinsings to the volumetric flask and dilute with water almost to volume. Allow the volumetric flask to reach room temperature (25°), then make up to volume with water and mix. Titrate a 50.0 ml aliquot with 0.1N ferrous ammonium sulfate using 2 or 3 drops of ortho-phenanthroline TS as the indicator and record the volume required as S in ml. Perform a blank determination and record the volume of 0.1N ferrous ammonium sulfate required as B in ml. Calculate the percentage of cellulose in the sample by the formula:

$$(B - S)\times \frac{338}{W}\%$$

Where: W is the weight of sample taken, in mg, corrected for loss on drying.

Infrared Spectrum



MICROCRYSTALLINE WAX

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 49th JECFA (1997) and published in FNP 52 Add 5 (1997). A group ADI of 0-20 mg/kg bw was established at the 44th JECFA (1995).

SYNONYMS	Petroleum wax; INS No. 905(c)
DEFINITION	Microcrystalline Wax is a refined mixture of solid, saturated hydrocarbons, mainly branched paraffin, obtained from petroleum
DESCRIPTION	Colourless or white, somewhat translucent, tasteless and odourless wax
FUNCTIONAL USES	Chewing gum base, protective coating, defoaming agent, surface finishing agent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, very slightly soluble in ethanol, sparingly soluble in diethyl ether and hexane
Refractive index (FNP 5)	n_D^{100}: 1.434 – 1.448
Infrared absorption	The infrared absorbance spectrum of the sample melted and prepared on a caesium or potassium bromide plate corresponds to the spectrum in the Appendix
PURITY	
Viscosity, 100°	Not less than 11 mm^2/sec See description under TESTS
Carbon number at 5% distillation point	Not more than 5% of molecules with carbon number less than 25 See description under TESTS
Average molecular weight	Not less than 500 See description under TESTS
Residue on ignition	Not more than 0.1% See description under TESTS
Colour	Passes test See description under TESTS
Sulfur	Not more than 0.4% See description under TESTS
Lead	Not more than 3 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described on FNP 5, "Instrumental methods".
Polycyclic aromatic hydrocarbons	The sample shall meet the following ultraviolet absorbance limits when subjected to the analytical procedure described under the TESTS.

nm	max. absorbance per cm path length
280 - 289	0.15
290 - 299	0.12
300 - 359	0.08
360 - 400	0.02

TESTS

PURITY TESTS

Viscosity, 100°

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Use a viscometer of the glass capillary type, calibrated and capable of measuring kinematic viscosity with a repeatability exceeding 0.35% only in one case in twenty. Immerse the viscometer in a liquid bath at the temperature required for the test ± 0.1° ensuring that at no time of the measurement will any portion of the sample in the viscometer be less than 20 mm below the surface of the bath. Charge the viscometer with sample in a manner directed by the design of the instrument. Allow the sample to remain in the bath for about 30 min. Where the design of the viscometer requires it, adjust the volume of sample to the mark. Use pressure to adjust the head level of the sample to a position in the capillary arm of the instrument about 5 mm ahead of the first mark. With the sample flowing freely, measure, in seconds (±0.2 sec), the time required for the meniscus to pass from the first to the second timing mark. If the time is less than 200 s, select a viscometer with a capillary of smaller diameter and repeat the operation. Make a second measurement of the flow time. If two measurements agree within 0.2%, use the average for calculating the kinematic viscosity. If the measurements do not agree, repeat the determination after thorough cleaning and drying the viscometer.

Viscosity, 100° (mm^2/sec) = C x t

where
C = calibration constant of the viscometer (mm^2/s)
t = flow time (s)

Carbon number at 5% distillation point

(ASTM D 5442 See TEST for Viscosity, 100° for Copyright permission)

"Carbon number" is number of carbon atoms in a molecule. Determine the carbon number distribution of the sample by gas chromatography. Below is shown some typical working conditions for determination of up to carbon number 45.

Column	length (m)	25	30	15
	inside diameter (mm)	0.32	0.53	0.25
	stationary phase	DB-1 methyl silicone	RTX-1 methyl silicone	DB-5 5% phenyl methyl silicone
	film thickness (μm)	0.25	0.25	0.25
Carrier	gas	helium	helium	helium
	flow (ml/min)	1.56	5.0	2.3
Linear velocity (cm/sec)		33	35	60
Temperature program				
	initial temperature	80°	80°	80°
	rate (°/min)	10	8	5
	final temperature	380°	340°	350°
Injection technique		cool on-column	cool on-column	cool on-column
Detector		FID	FID	FID
	temperature	380°	340°	375°
Sample size (μl)		1.0	1.0	1.0

NOTE: By optimizing the length of separation column and/or column temperature, waxes with carbon number higher than 45 can also be included.

Standards for calibration and identification:
Standard samples of normal paraffins covering the carbon number range of the sample of purity greater than 95%.

Linearity standard:
Prepare a weighed mixture of n-paraffins covering the range between C_{16} to C_{65} and dissolve the mixture in cyclohexane. Use approximately equal amounts of each of the paraffins weighed with 1% accuracy. Solutions of 0.01 % (w/w) may be used. It is not necessary to include every n-paraffin in this mixture so long as it contains C_{16}, C_{44}, (C_{60} if determination of higher carbon numbers is relevant) and at least one of every fourth n-paraffin. This standard must be capped tightly to prevent solvent loss.

Internal standard solution:
Prepare a stock solution containing 0.5% (w/w) n-C_{16} in n-hexane. (minimum purity of 98%) by accurately weighing approximately 0.4 g n-C_{16} into a 100 ml volumetric flask. Add 100 ml of cyclohexane and reweigh. Record the mass of n-C_{16} (W_{ISTD}) to within 0.001 g and the mass of the stock solution (Ws) to within 0.1 g. Prepare a dilute solution of internal standard by diluting one part of stock solution with 99 parts of cyclohexane. Calculate the concentration of internal standard using the following equation:

$$C_{INST} = \frac{W_{ISTD}}{Ws} \times \frac{100}{100} \; \% \, (w/w)$$

Where:
C_{INST} = concentration of n-C_{16} in the internal standard dilute solution in % (w/w)
W_{ISTD} = weight of n-C_{16} used for the stock solution in g.
Ws = Weight of the stock solution in g

Check of solvent blank:
Inject 1 µl of the solvent. No peaks must be detected within the retention time range over which the wax elutes.

Column resolution:
Inject 1 µl of a solution of 0.05 % each of n-C_{20} and n-C_{24} in cyclohexane. The column resolution R not be less than 30 as calculated by the following equation:

$$R = \frac{2d}{1.699\,(W1 + W2)}$$

Where
d = the distance in mm between the peak maxima of n-C_{20} and n-C_{24}
W1 = the peak with in mm of half height of n-C_{20}
W2 = the peak with in mm of half height of n-C_{24}

Linearity:
Analyze the linearity standard. The calculated mass response factors relative to hexadecane must be between 0.90 and 1.10.

Retention time repeatability:
Analyze the linearity standard in duplicate. The retention times for duplicate analysis must not differ more than 0.10 min between duplicate runs.

Calibration for n-paraffin identification:
Determine the retention time of each n-paraffin in the range from C_{16} to C_{44} (or C_{60} if determination of higher carbon numbers is relevant) by injecting small amounts of each paraffin either separately or in known mixtures.

Sampling:
Heat the sample to 10° above the temperature at which the wax is completely molten. Mix well by stirring.. Using a clean eyedropper, transfer a few drops to the surface of a

clean sheet of aluminium foil, allow to solidify and break into pieces. Aluminium foil usually contains a thin film of oil from processing. This oil must be removed by rinsing the foil with solvents such as hexane or mineral spirits, prior to use.

Procedure:
Accurately weigh about 0.0100 g of the sample (W_{sample}) obtained as described under sampling into a glass vial of approximately 15 ml capacity. Add approximately 12 ml of dilute internal standard solution, cap the vial and determine the exact weight of the added dilute internal standard solution (W_{INSTD}). Agitate the vial until the wax is completely dissolved using gentle heating if necessary.

Inject 0.5 to 1.0 μl of the sample solution. Record the chromatogram and store the detector signal. The peak from the internal standard must be completely resolved from the wax sample area. Based on the retention time as obtained under Calibration for n-paraffin identification, identify the normal paraffin peaks. Using a vertical drop to a horizontal baseline construction (see Figure 1), integrate the detector signal. Sum the area of all the peaks of each carbon number. By convention, the peaks assigned the carbon number n are those that elute between the valley immediately following the normal paraffin peak (C_{n-1}) and the corresponding valley following the next normal paraffin peak (C_n).

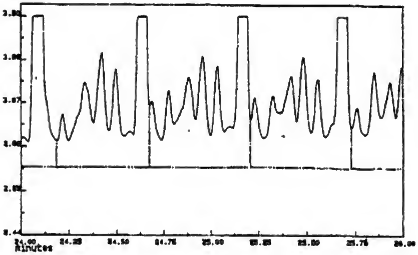


Figure 1. Carbon number summation (vertical drop to horizontal baseline)

Calculation:
For each carbon number, calculate the content in % (w/w) by using the following equation:

$$C_i = \frac{A_i}{A_{ISTD}} \times RRF_i \times \frac{W_{ISTD}}{W_{sample}} \times C_{ISTD}$$

Where
C_i = content in % (w/w) of hydrocarbons with carbon number i
A_i = area sun of hydrocarbons with carbon number I
A_{ISTD} = the area of n-C_{16} internal standard peak
RRFi = the response factor relative to n-C_{16}
W_{INSTD} = the weight of dilute internal standard solution
Wsample = the weight of wax sample
C_{ISTD} = the concentration of n-C_{16} in the dilute internal standardsolution

The combined contents of components with carbon number less than 25 is not more than 5%.

Average molecular weight

Using the carbon number distribution obtained in the test for "Carbon number at 5% distillation point" calculate the average molecular weight by the following formula:

Average molecular weight =

$$\frac{\sum_{i=17}^{i=i} C_i\,(14i+2)}{100}$$

where
i = the carbon number
C_i = the content in % of components having a carbon number of i

Residue on ignition

Accurately weigh about 2 g of the sample in a tared porcelain or platinum dish and heat over a flame. The sample volatilizes without emitting an acrid odour. Ignite to not exceeding a very dull redness until free from carbon. Cool in a desiccator and weigh.

Colour

Melt about 10 g of the sample on a steam bath, and pour 5 ml of the liquid into a clear-glass, 16 x 150-mm bacteriological test tube: the warm, melted liquid is not darker than a solution made by mixing 3.8 ml of ferric chloride TS (FNP 5) and 1.2 ml of cobaltous chloride TS (FNP 5) in a similar tube, the comparison of the two being made in reflected light against a white background, the tubes being held directly against the background at such an angle that there is no fluorescence.

Sulfur

(ASTM D 2622 See TEST for Viscosity, 100° for Copyright permission)

Determine by X-ray spectrometry using the following conditions:

Apparatus:
- X-ray spectrograph, equipped for soft ray detection in the 537 Å range
- Optical path of helium
- Pulse height analyzer or other means of energy discrimination
- Detector designed for detection of long wavelength X-rays
- Analyzing crystal suitable for the dispersion of sulfur Kα X-rays within the angular range of the spectrometer employed. Pentaerythritol and germanium are the most popular although less reflective materials such as EDDT, ADP and quartz may be used.
- X-ray tube of exiting sulfur Kα radiation.
- X-ray tube with tungsten, platinum or chromium target

Sensitivity standards:
Liquid petroleum materials containing sulfur in concentrations approximately in the middle of the calibration graph used for the test.

Calibration standards
Prepare calibration standards by careful weight dilution of di-n-butyl sulfide (high purity standard with a certified analysis, manufactured especially as a calibration material for this method, available from Philips Petroleum Co., Bartlesville, OK, USA) with white oil (containing less than 5 mg/kg). Exact standards of approximately 0.100, 0.250, 0.500 and 1.0 % (w/w) should be prepared.

Calibration curve:
Measure the net emitted sulfur radiation from each of the calibration standards. Plot the intensity, in terms of net counts per sec, against sulfur concentration.

To maintain the validity of the calibration curve with slight changes in the instruments sensitivity, measure the sensitivity standard at frequent intervals during the course of the days run. Establish the counting rate of this standard by measuring its intensity at frequent intervals during the preparation of the calibration curve. Calculate the correction factor for changes in daily instrument sensitivity by using the following equation:

$$F = \frac{A}{B}$$

Where
A = the counting rate of the sensitivity standard determined at the time of calibration
B = the counting rate of the sensitivity standard determined at the time of analysis

Procedure:
Place the sample in an appropriate cell. Although sulfur radiation will penetrate through only a small distance in the sample, scatter from the sample cup and the sample may vary to such an extend that a specific amount or a minimum amount of the sample must be used.

Place the sample in the X-ray beam and allow the X-ray optical atmosphere to come to equilibrium. Determine the intensity of the sulfur Kα radiation at 5.373 Å by making counting rate measurements at the precise angular settings for this wavelength. Measure background count-rate at 5.190 Å.

Calculation:
Calculate the content of sulfur in the sample using the following equation:

$$R = \left[\frac{C_K}{S_1} - \frac{C_B \times F'}{S_2} \right] \times F$$

R = the corrected net counting rate
C_K = total counts collected at 5.373 Å for the sample
S_1 = the time in sec required to collect C_K counts
C_B = total counts collected at 5.190 Å for background
S_2 = the time in sec required to collect C_B counts
F' = count-rate at 5.373 Å / count-rate at 5.190 Å for a sample not containing sulfur
F = the correction factor for changes in daily instrument sensitivity

Using the corrected net counting rate, read the sulfur concentration from the calibration curve.

Polycyclic aromatic hydrocarbons

General Instructions

Because of the sensitivity of the test, the possibility of errors arising from contamination is great. It is of the greatest importance that all glassware be scrupulously cleaned to remove all organic matter such as oil, grease, detergent residues, etc. Examine all glassware, including stoppers and stopcocks, under ultraviolet light to detect any residual fluorescent contamination. As a precautionary measure it is a recommended practice to rinse all glassware with purified isooctane immediately before use. No grease is to be used on stopcocks or joints. Great care to avoid contamination of wax samples in handling and to assure absence of any extraneous material arising from inadequate packaging is essential. Because some of the polynuclear hydrocarbons sought in this test are very susceptible to photo-oxidation, the entire procedure is to be carried out under subdued light.

Apparatus

- Separatory funnels: 250-ml, 500-ml, 1,000-ml, and preferably 2000-ml capacity, equipped with tetrafluoroethylene polymer stopcocks.
- Reservoir: 500 ml capacity, equipped with a 24/40 standard taper male fitting at the bottom and a suitable balljoint at the top for connecting to the nitrogen supply. The male fitting should be equipped with glass hooks.
- Chromatographic tube: 180 mm in length, inside diameter to be 15.7 mm ± 0.1 mm, equipped with a coarse, fritted-glass disc, a tetrafluoroethylene polymer stopcock, and a female 24/40 standard tapered fitting at the opposite end. (Overall length of the column with the female joint is 235 mm). The female 24/40 standard tapered fitting at the opposite end.
- Disc: Tetrafluoroethylene polymer 2-inch diameter disc approximately 3/16-inch thick

with a hole bored in the center to closely fit the stem of the chromatographic tube.

- Heating jacket: Conical, for 500-ml separatory funnel. (Used with variable transformer heat control).
- Suction flask: 250-ml or 500-ml filter flask.
- Condenser: 24/40 joints, fitted with a drying tube, length optional.
- Evaporation flask (optional): 250-ml or 500-ml capacity all-glass flask equipped with standard taper stopper having inlet and outlet tubes permitting passage of nitrogen across the surface of the liquid to be evaporated.
- Vacuum distillation assembly: All glass (for purification of dimethyl sulfoxide); 2 litre distillation flask with heating mantle; Vigreaux vacuum-jacketed condenser (or equivalent) about 45 cm in length and distilling head with separable cold finger condenser. Use of tetrafluoroethylene polymer sleeves on the glass joints will prevent freezing. Do not use grease on stopcocks or joints.
- Spectrophotometric cells: Fused quartz cells, optical path length in the range of 5.000 ± 0.005 cm; also for checking spectrophotometer performance only, optical path length in the range 1.000 ± 0.005 cm. With distilled water in the cells, determine any absorbance differences.
- Spectrophotometer: Spectral range 250-400 nm with spectral slit width of 2 nm or less, under instrument operating conditions for these absorbance measurements, the spectrophotometer shall also meet the following performance requirements:

Absorbance repeatability:	±0.01 at 0.4 absorbance
Absorbance accuracy:	±0.05 at 0.4 absorbance
Wavelength repeatability:	±0.2 nm
Wavelength accuracy:	±1.0 nm

- Nitrogen cylinder: Water-pumped or equivalent purity nitrogen in cylinder equipped with regulator and valve to control flow at 5 p.s.i.g.

Reagents and materials

- Organic solvents: All solvents used throughout the procedure shall meet the specifications and tests described in this specification. The isooctane, benzene, acetone, and methyl alcohol designated in the list following this paragraph shall pass the following test:

  To the specified quantity of solvent in a 250-ml Erlenmeyer flask, add 1 ml of purified n-hexadecane and evaporate on the steam bath under a stream of nitrogen (a loose aluminium foil jacket around the flask will speed evaporation). Discontinue evaporation when not over 1 ml of residue remains. (To the residue from benzene add a 10 ml portion of purified isooctane, reevaporate, and repeat once to insure complete removal of benzene).

  Alternatively, the evaporation time can be reduced by using the optional evaporation flask. In this case the solvent and n-hexadecane are placed in the flask on the steam bath, the tube assembly is inserted, and a stream of nitrogen is fed through the inlet tube while the outlet tube is connected to a solvent trap and vacuum line in such a way as to prevent any flow-back of condensate into the flask.

  Dissolve the 1 ml of hexadecane residue in isooctane and make to 25 ml volume. Determine the absorbance in the 5 cm path length cells compared to isooactane as reference. The absorbance of the solution of the solvent residue (except for methyl alcohol) shall not exceed 0.01 per cm path length between 280 and 400 nm. For methyl alcohol this absorbance value shall be 0.00.

- Isooctane (2,2,4-trimethylpentane): Use 180 ml for the test described in the preceding paragraph. Purify, if necessary, by passage through a column of activated silica gel (Grade 12, Davison Chemical Company, Baltimore, Maryland. or equivalent) about 90 cm in length and 5 cm to 8 cm in diameter.
- Benzene, reagent grade: Use 150 ml for the test. Purify, if necessary, by distillation or otherwise.
- Acetone, reagent grade: Use 200 ml for the test. Purify, if necessary, by distillation.

- Eluting mixtures:
  1. 10% benzene in isooctane: Pipet 50 ml of benzene into a 500-ml glass-stoppered volumetric flask and adjust to volume with isooctane, with mixing.
  2. 20% benzene in isooctane: Pipet 50 ml of benzene into a 250-ml glass-stoppered volumetric flask, and adjust to volume with isooctane, with mixing.
  3. Acetone-benzene-water mixture: Add 20 ml of water to 380 ml of acetone and 200 ml of benzene, and mix.
- n-Hexadecane, 99% olefin-free: Dilute 1.0 ml of n-hexadecane to 25 ml with isooctane and determine the absorbance in a 5-cm cell compared to isooctane as reference point between 280-400 nm. The absorbance per centimeter path length shall not exceed 0.00 in this range. Purify, if necessary, by percolation through activated silica gel or by distillation.
- Methyl alcohol, reagent grade: Use 10.0 ml of methyl alcohol. Purify, if necessary, by distillation.
- Dimethyl sulfoxide: Pure grade, clear, water-white, m.p. 18° minimum. Dilute 120 ml of dimethyl sulfoxide with 240 ml of distilled water in a 500-ml separatory funnel, mix and allow to cool for 5-10 min. Add 40 ml of isooctane to the solution and extract by shaking the funnel vigourously for 2 min. Draw off the lower aqueous layer into a second 500 ml separatory funnel and repeat the extraction with 40 ml of isooctane. Draw off and discard the aqueous layer. Wash each of the 40 ml extractives three times with 50 ml portions of distilled water. Shaking time for each wash is 1 min. Discard the aqueous layers. Filter the first extractive through anhydrous sodium sulfate prewashed with isooctane (see Sodium sulfate under "Reagents and Materials" for preparation of filter), into a 250-ml Erlenmeyer flask, or optionally into the evaporating flask. Wash the first separatory funnel with the second 40 ml isooctane extractive, and pass through the sodium sulfate into the flask. Then wash the second and first separatory funnels successively with a 10 ml portion of isooctane, and pass the solvent through the sodium sulfate into the flask. Add 1 ml of n-hexadecane and evaporate the isooctane on the steam bath under nitrogen. Discontinue evaporation when not over 1 ml of residue remains. To the residue, add a 10 ml portion of isooctane and reevaporate to 1 ml of hexadecane. Again, add 10 ml of isooctane to the residue and evaporate to 1 ml of hexadecane to insure complete removal of all volatile materials. Dissolve the 1 ml of hexadecane in isooctane and make to 25 ml volume. Determine the absorbance in 5 cm path length cells compared to isooctane as reference. The absorbance of the solution should not exceed 0.02 per cm path length in the 280-400 nm range. (Note - Difficulty in meeting this absorbance specification may be due to organic impurities in the distilled water. Repetition of the test omitting the dimethyl sulfoxide will disclose their presence. If necessary to meet the specification, purify the water by redistillation, passage through an ion-exchange resin, or otherwise).

  Purify, if necessary, by the following procedure: To 1.5 L of dimethyl sulfoxide in a 2 l glass-stoppered flask, add 6.0 ml of phosphoric acid and 50 g of Norit A (decolorizing carbon, alkaline) or equivalent. Stopper the flask, and with the use of a magnetic stirrer (tetrafluoroethylene polymer coated bar) stir the solvent for 15 min. Filter the dimethyl sulfoxide through four thicknesses of fluted paper (18.5 cm) (Schleicher & Schuell No. 597, or equivalent). If the initial filtrate contains carbon fines, refilter through the same filter until a clear filtrate is obtained. Protect the sulfoxide from air and moisture during this operation by covering the solvent in the funnel and collection flask with a layer of isooctane. Transfer the filtrate to a 2-l separatory funnel and draw off the dimethyl sulfoxide into the 2-l distillation flask of the vacuum distillation assembly and distill at approximately 3 mm Hg pressure or less. Discard the first 200 ml fraction of the distillate and replace the distillate collection flask with a clean one. Continue the distillation until approximately 1 litre of the sulfoxide has been collected.

  At completion of the distillation, the reagent should be stored in glass-stoppered bottles since it is very hygroscopic and will react with some metal containers in the presence of air.

- Phosphoric acid, 85% reagent grade
- Sodium borohydride, 98%
- Magnesium oxide (Sea Sorb 43, Food Machinery Company, Westvaco Division, distributed by chemical supplier firms, or equivalent): Place 100 g of the magnesium

oxide in a large beaker, add 700 ml of distilled water to make a thin slurry, and heat on a steam bath for 30 min with intermittent stirring. Stir well initially to insure that all the absorbent is completely wetted. Using a Buchner funnel and a filter paper* of suitable diameter, filter with suction. Continue suction until water no longer drips from the funnel. Transfer the absorbent to a glass trough lined with aluminium foil (free from rolling oil). Break up the magnesia with a clean spatula and spread out the absorbent on the aluminium foil in a layer about 1-2 cm thick. Dry at 160±1° for 24 h. Pulverize the magnesia with mortar and pestle. Sieve the pulverized absorbent between 60-180 mesh. Use the magnesia retained on the 180-mesh sieve.

- Celite 545 (Johns-Manville Company, diatomaceous earth, or equivalent)
- Magnesium oxide-Celite 545 mixture (2+1) by weight: Place the magnesium oxide (60-180 mesh) and the Celite 545 in 2 to 1 proportions, respectively, by weight in a glass-stoppered flask large enough for adequate mixing. Shake vigorously for 10 min. Transfer the mixture to a glass trough lined with aluminium foil (free from rolling oil) and spread it out on a layer about 1 to 2 cm thick. Reheat the mixture at 160±1° for 2 h, and store in a tightly closed flask.
- Sodium sulfate, anhydrous, reagent grade, preferably in granular form: For each bottle of sodium sulfate reagent used, establish as follows the necessary sodium sulfate prewash to provide such filters required in the method: Place approximately 35 g of anhydrous sodium sulfate in a 30 ml coarse, fritted-glass funnel or in a 65 ml filter funnel with glass wool plug; wash with successive 15 ml portions of the indicated solvent until a 15 ml portion of the wash shows 0.00 absorbance per cm path length between 280 nm and 400 nm when tested as prescribed under "Organic solvents." Usually three portions of wash solvent are sufficient.

Procedure

Before proceeding with the analysis of a sample, determine the absorbance in a 5 cm path cell between 250 nm and 400 nm for the reagent blank by carrying out the procedure, without a wax sample, at room temperature, recording the spectra after the extraction stage and after the complete procedure as precribed. The absorbance per centimeter path length following the extraction stage should not exceed 0.040 in the wavelength range from 250 to 400 nm; the absorbance per cm path length following the complete procedure should not exceed 0.070 in the wavelength range from 250 to 299 nm, inclusive, nor 0.045 in the wavelength range from 300 nm to 400 nm. If in either spectrum the characteristic benzene peaks in the 250-260 nm region are present, remove the benzene by the procedure under "Organic solvents" and record absorbance again.

Place 300 ml of dimethyl sulfoxide in a 1liter separatory funnel and add 75 ml of phosphoric acid. Mix the contents of the funnel and allow to stand for 10 min. (The reaction between the sulfoxide and the acid is exothermic. Release pressure after mixing, then keep funnel stoppered). Add 150 ml of isooctane and shake to preequilibrate the solvents. Draw off the individual layers and store in glass-stoppered flasks.

Place a representative 1 kg sample of wax, or if this amount is not available, the entire sample, in a beaker of a capacity about three times the volume of the sample and heat with occasional stirring on a steam bath until the wax is completely melted and homogenous. Weigh four 25 ± 0.2 g portions of the melted wax in separate 100 ml beakers. Reserve three of the portions for later replicate analyses as necessary. Pour one weighed portion immediately after remelting (on the steam bath) into a 500 ml separatory funnel containing 100 ml of the preequilibrated sulfoxide-phosphoric acid mixture that has been heated in the heating jacket at a temperature just high enough to keep the wax melted. (Note: In preheating the sulfoxide-acid mixture, remove the stopper of the separatory funnel at intervals to release the pressure).

Promptly complete the transfer of the sample to the funnel in the jacket with portions of the preequilibrated isooctane, warming the beaker, if necessary, and using a total volume of just 50 ml of the solvent. If the wax comes out of solution during these operations, let the stoppered funnel remain in the jacket until the wax redissolves. (Remove stopper from the funnel at intervals to release pressure).

When the wax is in solution, remove the funnel from the jacket and shake it vigorously for 2 min. Set up three 250 ml separatory funnels with each containing 30 ml of preequilibrated isooctane. After separation of the liquid phases, allow to cool until the main portion of the wax-isooctane solution begins to show a precipitate. Gently swirl the funnel when precipitation first occurs on the inside surface of the funnel to accelerate this process. Carefully draw off the lower layer, filter it slowly through a thin layer of glass wool fitted loosely in a filter funnel into the first 250 ml separatory funnel, and wash in tandem with the 30 ml portions of isooctane contained in the 250 ml separatory funnels. Shaking time for each wash is 1 min. Repeat the extraction operation with two additional portions of the sulfoxide-acid mixture, replacing the funnel in the jacket after each extraction to keep the wax in solution and washing each extractive in tandem through the same three portions of isooctane.

Collect the successive extractives (300 ml total) in a separatory funnel (preferably 2 liter), containing 480 ml of distilled water, mix, and allow to cool for a few minutes after the last extractive has been added. Add 80 ml of isooctane to the solution and extract by shaking the funnel vigorously for 2 min. Draw off the lower aqueous layer into a second separatory funnel (preferably 2 litre) and repeat the extraction with 80 ml of isooctane. Draw off and discard the aqueous layer. Wash each of the 80 ml extractives three times with 100 ml portions of distilled water. Shaking time for each wash is 1 min. Discard the aqueous layers. Filter the first extractive through anhydrous sodium sulfate prewashed with isooctane (see Sodium Sulfate under "Reagents and Materials" for preparation of filter) into a 250-ml Erlenmeyer flask (or optionally into the evaporation flask). Wash the first separatory funnel with the second 80 ml isooctane extractive and pass through the sodium sulfate. Then wash the second and first separatory funnels successively with a 20 ml portion of isooctane and pass the solvent through the sodium sulfate into the flask. Add 1 ml of n-hexadecane and evaporate the isooctane on the steam bath under nitrogen. Discontinue evaporation when not over 1 ml of residue remains. To the residue, add a 10 ml portions of isooctane, reevaporate to 1 ml of hexadecane, and repeat this operation once more.

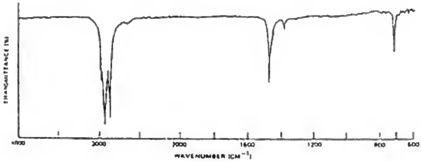
Quantitatively transfer the residue with isooctane to a 25 ml volumetric flask, make to volume, and mix. Determine the absorbance of the solution in the 5 cm path length cells compared to isooctane as reference between 280-400 nm (take care to lose none of the solution in filling the sample cell). Correct the absorbance values for any absorbance derived from reagents as determined by carrying out the procedure without a wax sample. If the corrected absorbance does not exceed the limits prescribed in the Characteristics, the wax meets the ultraviolet absorbance specifications. If the corrected absorbance per centimeter path length exceeds the limits prescribed in the Characteristics, proceed as follows:

Quantitatively transfer the isooctane solution to a 125 ml flask equipped with 24/40 joint and evaporate the isooctane on the steam bath under a stream of nitrogen to a volume of 1 ml of hexadecane. Add 10 ml of methyl alcohol and approximately 0.3 g of sodium borohydride (Minimize exposure of the borohydride to the atmosphere. A measuring dipper may be used). Immediately fit a water-cooled condenser equipped with a 24/40 joint and with a drying tube into the flask, mix until the borohydride is dissolved, and allow to stand for 30 min at room temperature, with intermittent swirling. At the end of this period, disconnect the flask and evaporate the methyl alcohol on the steam bath under nitrogen until the sodium borohydride begins to come out of the solution. Then add 10 ml of isooctane and evaporate to a volume of about 2-3 ml. Again, add 10 ml of isooctane and concentrate to a volume of approximately 5 ml. Swirl the flask repeatedly to assure adequate washing of the sodium borohydride residues.

Fit the tetrafluoroethylene polymer disc on the upper part of the stem of the chromatographic tube, then place the tube with the disc on the suction flask and apply the vaccum (approximately 135 mm Hg pressure). Weigh out 14 g of the 2+1 magnesium oxide-Celite 545 mixture and pour the adsorbent mixture into the chromatographic tube in approximately 3 cm layers. After the addition of each layer, level off the top of the adsorbent with a flat glass rod or metal plunger by pressing down firmly until the adsorbent is well packed. Loosen the topmost few ml of each adsorbent layer with the end of a metal rod before the addition of the next layer. Continue packing in this manner until all the 14 g of the adsorbent is added to the tube. Level off the top of the adsorbent by pressing down firmly with a flat glass rod or metal plunger to make the depth of the adsorbent bed approximately 12.5 cm in depth. Turn off the vacuum and remove the suction flask. Fit the 500 ml reservoir onto the top of the chromatographic column and prewet the column by passing 100 ml of isooctane through the column. Adjust the nitrogen pressure so that the rate of descent of the isooctane coming off of the column is between 2-3 ml per min. Discontinue pressure just before the last of the isooctane reaches the level of the adsorbent. (Caution: Do not allow the liquid level to recede below the adsorbent level at any time). Remove the reservoir and decant the 5 ml isooctane concentrate solution onto the column and with slight pressure again allow the liquid level to recede to barely above the adsorbent level. Rapidly complete the transfer similarly with two 5 ml portions of isooctane, swirling the flask repeatedly each time to assure adequate washing of the residue. Just before the final 5 ml wash reaches the top of the adsorbent, add 100 ml of isooctane to the reservoir and continue the percolation at the 2-3 ml per minute rate. Just before the last of the isooctane reaches the adsorbent level, add 100 ml of 10% benzene in isooctane to the reservoir and continue the percolation at the aforementioned rate. Just before the solvent mixture reaches adsorbent level, add 25 ml of 20% benzene in isooctane to the reservoir and continue the percolation at 2-3 ml per minute until all this solvent mixture has been removed from the column. Discard all the elution solvents collected up to this point. Add 300 ml of the acetone-benzene-water mixture to the reservoir and percolate through the column to elute the polynuclear compounds. Collect the eluate in a clean 1-l separatory funnel. Allow the column to drain until most of the solvent mixture is removed. Wash the eluate three times with 300 ml portions of distilled water, shaking well for each wash. (The addition of small amounts of sodium chloride facilitates separation). Discard the aqueous layer after each wash. After the final separation, filter the residual benzene through anhydrous sodium sulfate prewashed with benzene (see Sodium sulfate under "Reagents and Materials" for preparation of filter) into a 250-ml Erlenmeyer flask (or optionally into the evaporation flask). Wash the separatory funnel with two additional 20 ml portions of benzene which are also filtered through the sodium sulfate. Add 1 ml of n-hexadecane and completely remove the benzene by evaporation under nitrogen, using the special procedure to eliminate benzene as previously described under, "Organic Solvents". Quantitatively transfer the residue with isooctane to a 25 ml volumetric flask and adjust the volume. Determine the absorbance of the solution in the 5 cm path length cells compared to isooctane as reference between 250 - 400 nm. Correct for any absorbance derived from the reagents as determined by carrying out the procedure without a wax sample. If either spectrum shows the characteristic benzene peaks in the 250 - 260 nm region, evaporate the solution to remove benzene by the procedure under "Organic Solvents". Dissolve the residue, transfer quantitatively, and adjust to volume in isooctane in a 25 ml volumetric flask. Record the absorbance again. If the corrected absorbance does not exceed the limits prescribed in the Characteristics the wax meets the ultraviolet absorbance specifications.

Appendix

Infrared spectrum **Microcrystalline wax**



NITROUS OXIDE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 29th JECFA (1985) and published in FNP 34 (1986) and in FNP 52 (1992). An ADI "Acceptable" was established at the 29th JECFA (1985).

SYNONYMS	Nitrogen oxide, Dinitrogen monoxide; INS No. 942

DEFINITION

Chemical names	Dinitrogen monoxide
C.A.S. number	10024-97-2
Chemical formula	N_2O
Formula weight	44.01
Assay	Not less than 97% (v/v)
DESCRIPTION	Colourless, odourless gas
FUNCTIONAL USES	Propellant, antioxidant, packaging gas, foaming agent

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)	1 volume dissolves in 1.5 volumes of water (20°, 760 mm Hg)
Flame test	A glowing splinter of wood in contact with nitrous oxide bursts into flame (distinction from nitrogen).
Pyrogallol test	Passes test (distinction from oxygen). See description under TESTS

PURITY

Carbon monoxide	Not more than 10 µl/l See description under TESTS
Nitric oxide and nitrogen dioxide	Not more than 5 µl/l See description under TESTS
Halogens and hydrogen sulfide	Not more than 5 µl/l See description under TESTS
Arsine and phosphine	Passes test See description under TESTS

TESTS

IDENTIFICATION TESTS

Pyrogallol test	Collect about 100 ml of the gas under test in a 100-ml tube fitted at the top with a stopcock. Open the stopcock, and quickly add a freshly prepared solution of 500 mg of pyrogallol in 2 ml of water and a freshly prepared solution of 12 g of potassium hydroxide in 8 ml of water. Immediately close the stopcock, and mix. The gas is not absorbed and the solution does not become brown .
PURITY TESTS	NOTE: For the following tests keep the cylinder of gas from which the sample is taken

at room temperature for not less than 6 h before carrying out the tests. In all the tests the cylinder is kept in the vertical position with the outlet valve uppermost when delivering the gas. Pass the gas at a steady rate of 4 l/h unless otherwise stated and carry out the tests or calculate the results with reference to the gas at 20° and 760 mm Hg).

Carbon monoxide

Principle: Carry out the test on the first portion of gas issuing from the cylinder. Use 5.0 l of the nitrous oxide in the test and 5.0 l of carbon monoxide-free air as the control. The difference between the volumes of 0.002 N sodium thiosulfate used in the two titrations is not greater than 0.5 ml.

Apparatus: The apparatus consists of the following parts connected in series:
- U-tube containing anhydrous silica gel impregnated with chromium trioxide.
- Scrubber bottle (dreschel type) containing 100 ml of a 40% w/v solution of potassium hydroxide.
- U-tube containing pellets of potassium hydroxide.
- U-tube containing phosphorous pentoxide dispersed on previously granulated, fused pumice.
- Tube containing recrystallized iodic anhydride (I_2O_5) in granules, previously dried at 200° and kept at a temperature of 120°. The iodic anhydride is packed in the tube in 1 cm columns separated by 1 cm columns of glass wool to give an effective length of 5 cm.
- Flask containing 2.0 ml of potassium iodide TS and 3 drops of starch solution TS.

Procedure

Flush the apparatus with 5.0 l of carbon dioxide-free air and, if necessary, discharge the blue colour in the iodide solution by adding the smallest necessary quantity of freshly prepared 0.002 N sodium thiosulfate. Continue flushing until not more than 0.045 ml of 0.002 N sodium thiosulfate is required after passing 5.0 l of carbon dioxide-free air.

Pass the gas from the cylinder through the apparatus, using the volume and the rate of flow prescribed in the monograph. Flush the last traces of liberated iodine into the reaction flask by passing through the apparatus 1.0 l of carbon monoxide-free air. Titrate the liberated iodine with 0.002 N sodium thiosulfate.

Carry out a blank assay under the same conditions, using the carbon monoxide-free gas prescribed in the monograph. The difference between the volumes of 0.002 N sodium thiosulfate used in the two titrations is not greater than the limit prescribed in the monographs.

Nitric oxide and nitrogen dioxide

Principle: Carry out the test after the 5 l used in the test for carbon monoxide have been released from the cylinder. Pass the gas, at a rate of 15.0 l/h, through a solution containing 2.5% w/v of potassium permanganate and 1.2% v/v of sulfuric acid into an evacuated gas sampling tube of 1 l nominal capacity and fill to a pressure about 50 mm below that of the atmosphere, measured on a mercury manometer. Calculate the volume of gas at 20° and 760 mm Hg.

Sulfanilic acid/naphthylenediamine TS
- Solution I: Dissolve 2 g of sulfanilic acid TS in a mixture of 10 ml of glacial acetic acid and 180 ml of water.
- Solution II: Dissolve 0.2 g of naphthylenediamine dihydrochloride in 10 ml of a 50% v/v glacial acetic acid solution heating gently and dilute to 200 ml with water.

Mix 9 volumes of Solution I with 1 volume of Solution II.

Procedure

Introduce 20.0 ml of sulfanilic acid/naphthylenediamine TS into the sampling tube by dipping the end into a dish containing the mixture and carefully opening the tap. Shake the tube and allow to stand for 10 min with occasional shaking. Prepare the reference solution by adding 0.25 ml of 0.00308% w/v sodium nitrite solution to 20.0 ml of the sulfanilic acid/naphthylenediamine TS. Measure the absorbance of a 1 cm layer of the resulting solutions at 550 nm and correct the result to 1.0 l of the gas at 20° and 760 mm Hg. The extinction of 1.0 l of the test substance is not greater than that of the reference solution.

Halogens and hydrogen sulfide

NOTE: For the following test pass the gas into a closed, flat-bottomed glass cylinder fitted with (a) a delivery tube having an orifice of 1 mm internal diameter and reaching to 2 mm from the bottom of the cylinder and (b) an outlet tube. The delivery tube is immersed in the reagent to a depth of 12 to 14 cm.

Pass 10.0 l through 49 ml of water containing 1 ml of silver nitrate TS. The solution does not darken. After 5 min, any opalescene produced is not more intense than that obtained with a mixture of 1 ml of silver nitrate TS, 20 ml of chloride standard solution (5 mg of Cl per l), 0.15 ml of dilute nitric acid TS and sufficient water to make 50 ml of solution and left to stand for 5 min.

Arsine and phosphine

Silver DDC/Quinoline TS: Dissolve 50 mg of finely powdered silver nitrate in 100 ml of quinoline and add 0.2 g of silver diethyldithiocarbamate. The reagent should be freshly prepared.

Procedure: Pass 10.0 l at a rate of 1.0 l/min through a glass tube packed with lead acetate TS on cotton wool and a gas distribution head of the domed, sintered type, of porosity 100, into a tube of about 2.5 cm internal diameter, containing 5 ml of Silver DDC/Quinoline TS, the domed head being almost in contact with the bottom of the tube. The colour of the Silver DDC/Quinoline TS is not changed.

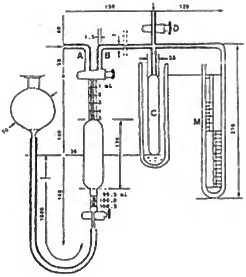
METHOD OF ASSAY

Use a gas burette (see Figure below) of 100 ml capacity having as its upper end a two-way tap connected to two capillaries, one of which (tube A) is used to introduce the gas into the apparatus, the other (tube B) connected to the condenser (C) and the manometer (M). The lower part of the gas burette has a one-way tap connected to a mercury reservoir by a rubber tube. The gas burette is graduated form 0 to 5 ml in tenths of a ml in the upper part and from 99.5 to 100.5 ml in tenths of a ml in the lower part. The capillary tube (B) is connected to a vertical capillary arm to form a four-way junction. The descending arm of the junction is connected to a condenser (C) of about 60 ml capacity. The right arm of the junction is connected to a mercury manometer (M). A tap (D) on the upper vertical arm of the junction opens to the air.

Close the three taps and immerse the condenser in liquid nitrogen, keeping the level slightly above the upper part of the condenser. By manipulating the two-way tap and the mobile reservoir create a partial vacuum in the apparatus, choosing an arbitrary pressure Po between 50 and 60 mm Hg, accurately measured. This pressure must remain constant for 10 min to demonstrate that the apparatus is gas-tight.

Open the two-way tap to tube (A) and completely fill the burette and tube (A) with mercury. Close the two-way tap. Connect a rubber tube to the exit valve of the nitrous oxide cylinder through a suitable pressure relieving device and pass a current of nitrous oxide through the rubber tube for 1 min. Whilst the gas is still flowing, connect the rubber tube to the end of tube (A) and immediately open the two-way tap to tube (A). Allow 100 ml of nitrous oxide to enter the burette by lowering the mercury reservoir. Close the two-way taps.

Raise the mercury reservoir slightly above the tube (A) and lower the level of the liquid nitrogen to the middle of the condenser. Carefully open the tap of the burette to connect with the condenser and allow the mercury to rise in the burette until it reaches the tap. Close the tap. Raise the level of the liquid nitrogen so as to totally immerse the condenser. Read the pressure and wait until it remains steady for 2 min.
Place the mercury reservoir in its bottom position, open the tap of the burette to make connection with the condenser. Move the mercury reservoir until the manometer reading is the same as the initial pressure Po. Close the tap of the burette and by means of the mercury reservoir bring the pressure of the gas in the burette to atmospheric pressure. The number of ml of gas represents the non-condensible volume in 100 ml of nitrous oxide. The volume of non-condensible gas must not exceed 3 ml. After each series of 10 determinations allow atmospheric air to enter by opening the tap (D), remove the liquid nitrogen from the condenser and allow the condenser to warm to room temperature.


150
170
D
60
1.5
A
B
38
C
M
270
1 ml
100
36
170
99.5 ml
100.0
100.5
140
1000
70

OXYSTEARIN
(Tentative)

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 20th JECFA (1976) and published in FNS 1B (1977) and in FNP 52 (1992). An ADI of 0-25 mg/kg bw was established at the 17th JECFA (1973).

Information on the levels of epoxides and suitable methods for the determination of epoxides is requested. Comments on other aspects of the monograph are invited. If no information is forthcoming before 1 May 2001, this monograph will be withdrawn.

SYNONYMS	INS No. 387
DEFINITION	A mixture of glycerides of partially oxidized stearic and other fatty acids; obtained by heating hydrogenated vegetable oil under controlled conditions
DESCRIPTION	Tan to light brown, fatty or wax-like substance
FUNCTIONAL USES	Crystallization inhibitor, sequestrant, antifoaming agent

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)	Soluble in ether and in hexane

PURITY

Refractive index (FNP 5)	Between 1.465 and 1.467 at 48° by the following procedure. Melt the sample, filter through filter paper and determine the refractive index at 48°.
Acid value (FNP 5)	Not more than 15 Use about 8 g of the sample weighed to the nearest mg.
Hydroxyl value (FNP 5)	Between 30 and 45 Use about 5 g of the sample weighed to the nearest mg
Iodine value (FNP 5)	Not more than 15 Use about 1 g of the sample weighed to the nearest mg
Saponification value (FNP 5)	Between 225 and 240 Use about 3 g of the sample weighed to the nearest mg
Unsaponifiable matter	Not more than 0.8% See description under TESTS
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Unsaponifiable matter	Accurately weigh about 5 g of the sample into a 250 ml round-bottomed flask. Add a solution of 2 g of potassium hydroxide in 40 ml of ethanol and boil gently under a reflux condenser for 1 h or until saponification is complete. Transfer the contents of the

flask to a glass-stoppered extraction cylinder (approximately 30 cm in height, 3.5 cm in diameter, and graduated at 40, 80 and 130 ml). Wash the flask with sufficient ethanol to make a volume of 40 ml in the cylinder, and complete the transfer with warm and then cold water until the total volume is 80 ml. Finally, wash the flask with a few ml of petroleum ether, add the washings to the cylinder, cool the contents of the cylinder to room temperature, and add 50 ml of petroleum ether.

Insert the stopper, shake the cylinder vigorously for at least 1 min, and allow both layers to become clear. Siphon the upper layer as completely as possible without removing any of the lower layer, collecting the ether fraction in a 500-ml separator. Repeat the extraction and siphoning at least six times with 50-ml portions of petroleum ether, shaking vigorously each time. Wash the combined extracts, with vigorous shaking, with 25-ml portions of 10% ethanol until the wash water is neutral to phenolphthalein and discard the washings. Transfer the ether extract to a tared beaker, and rinse the separator with 10 ml of ether, adding the rinsings to the beaker. Evaporate the ether on a steam bath just to dryness, and dry the residue to constant weight, preferably at 75-80° under vacuum of not more than 200 mm of Hg, or at 100° for 30 min. Cool in a desiccator, and weigh to obtain the uncorrected weight of unsaponifiable matter.

Determine the quantity of fatty acids in the residue as follows: Dissolve the residue in 50 ml of warm ethanol (containing phenolphthalein TS and previously neutralized with sodium hydroxide to a faint pink colour), and titrate with 0.02 N sodium hydroxide to the same colour. Each ml of 0.02 N sodium hydroxide is equivalent to 5.659 mg of fatty acids, calculated as oleic acid.

Subtract the calculated weight of fatty acids from the weight of the residue obtained to obtain the corrected weight of unsaponifiable matter in the sample.

PECTINASE FROM *ASPERGILLUS NIGER*, VAR.

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Not specified" was established at the 35th JECFA (1989).

SOURCES

Produced by the controlled fermentation of non-pathogenic and non-toxicogenic strains of *Aspergillus niger* and isolated from the growth medium.

ACTIVE PRINCIPLES

1. Pectinesterase (synonym: pectin methylesterase)
2. Polygalacturonase
3. Pectin lyase (synonym: pectin depolymerase)

SYSTEMATIC NAMES AND NUMBERS

1. Pectin pectylhydrolase (EC 3.1.1.11; C.A.S. No. 9025-98-3)
2. Poly (1,4-α-D-galacturonide)glycanohydrolase (EC 3.2.1.15; C.A.S. No. 9032-75-1)
3. Poly (methoxy-L-galacturonide) lyase (EC 4.2.2.10; C.A.S. No. 9033-35-6)

REACTIONS CATALYZED

1. Demethylation of pectin
2. Hydrolysis of 1,4-α-galacturonide linkages in pectin
3. Eliminative cleavage of pectin to give oligosaccharides

SECONDARY ENZYME ACTIVITIES

α-Amylase (1,4-α-D-glucan-glucanohydrolase, EC 3.2.1.1; C.A.S. No. 9000-90-2)
β-Glucanase (EC 3.2.1.6; C.A.S. No. 9074-99-1)
β-Glucosidase (EC 3.2.1.21; C.A.S. No. 9001-22-3)
Cellulase ((1,4-[1,3;1,4]-β-D-Glucan 4-glucano.-hydrolase; EC 3.2.1.4; C.A.S. No. 9012-54-8)
Xylanase (EC 3.2.1.32)

DESCRIPTION

Typically off-white to tan amorphous powders or tan to dark-brown liquids. The unformulated product is usually diluted and standardised with food grade glycerol, water and potassium chloride to obtain commercial products. Soluble in water and practically insoluble in ethanol and ether.

FUNCTIONAL USES

Enzyme preparation.
Used mostly to reduce viscosity, to improve filtration to clarify products, to avoid particle sedimentation and to prevent pectin gel formation in the manufacture of fruit juice and wine.

GENERAL SPECIFICATIONS

Must conform to the General Specifications for Enzyme Preparations used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7)

CHARACTERISTICS

IDENTIFICATION

Pectinase activity

The sample shows Pectinase activity
See description under TESTS

TESTS

Pectinase activity

Principle
This assay method is based on the enzymatic hydrolysis of pectin, the resulting galacturonic acid being determined spectrophotometrically at 235 nm. One unit of pectinase activity (PTA) causes an increase of 0.010 of absorbance per minute under the conditions of the assay (Pectin 0.5 %, pH 5.8 and 30°)

Apparatus:
Spectrophotometer set at 235 nm (if possible double beam type, preferably with reference automation and cuvett changer).
Water bath set at 30.0 ± 0.1°

Reagents and solutions:

Citrate buffer pH 5.8

35.6 g Disodium hydrogen phosphate ($Na_2HP0_4.2H_20$) are dissolved in 1000 ml of water (A). 21 g of Citric acid monohydrate are dissolved in 1000 ml of water (B). 57 ml of solution A and 43 ml of solution B are mix to obtain working buffer solution. pH can be adjusted to 5.8 by adding one of the aforesaid solutions.

Pectin substrate solution

0.5 g of pectin (pectin, such as Copenhagen Pectin X, 2955, or Sigma, P2157) are mashed with 2 ml ethanol in a beaker and stirred to homogenity with a magnetic stirrer. Slowly (allow 2 minutes for this step) add 80 ml of 0.1 M citrate buffer and continue stirring, avoiding foam formation. Measure pH and if necessary adjust to pH= 5.8 with solutions A or B respectively. Transfer solution to a volumetric flask and add 0.1 M citrate buffer up to 100 ml. Keep substrate solution cool over night (refrigerator). Next day centrifuge solution 10 minutes at 12000 x g.

Samples preparation

Weigh 0.5 g to 2 g of sample and dissolve with buffer solution into a volumetric flask. Fill up to 100 ml and transfer 3 ml of this solution to a next volumetric flask and fill up with buffer to 25 ml. Sample solutions have to be prepared immediately before analysis.

Standard enzyme solution

Dilute standard enzyme (such as Sigma P 9179, Rohapect D5L or equivalent) with known activity in buffer solution to give 12 PTA enzyme units per ml.

Procedure

Measurement of enzyme activity

Add 0.1 ml of sample or standard solution to 3.0 ml of substrate solution pre-warmed to 30 ± 0.1° for 5 min. After short mixing, the absorbance at 235 nm is registered each minute over 8 minutes using distilled water as blank. Determination is done in triplicate.

Calculation

Plot absorbance (sample-water blank) data as the abscissa and time of reaction as the ordinate. The slope of the extinction, ($\Delta A/\Delta t$), is determined in the linear section of the function. The linear part should encompass at least 5 minutes (6 data points). Delays of the enzyme reaction before the linear part (lag-phase) are not taken into account. Pectinase activity units is calculated as:

$$\text{Pectinase Activity, U / mg } = \frac{\Delta A_{235} / \Delta t}{0.01 \times C \times V}$$

Where:

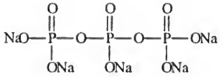
V = final reaction volume, ml (0.1 ml of sample or standard solution plus 3.0 ml of substrate solution)

C = final sample or standard concentration, mg/ml

The change in absorbance should not exceed 0.03 per min. Best values are within a range of 0.02 to 0.03.

PENTASODIUM TRIPHOSPHATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 20th JECFA (1976) and published in FNS 1B (1977) and in FNP 52 (1992). No ADI was established, but a group MTDI of 70 mg/kg bw, expressed as phosphorus from all food sources, was established at the 26th JECFA (1982).

SYNONYMS	Pentasodium tripolyphosphate, Sodium triphosphate, Sodium tripolyphosphate, Triphosphate; INS No. 451(i)
DEFINITION	
Chemical names	Pentasodium triphosphate, pentasodium tripolyphosphate
C.A.S. number	7758-29-4
Chemical formula	$Na_5O_{10}P_3 \cdot x\,H_2O$ (x = 0 or 6)
Structural formula	 $NaO{-}\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle ONa}{|}}{P}}{-}O{-}\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle ONa}{|}}{P}}{-}O{-}\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle ONa}{|}}{P}}{-}ONa$
Formula weight	Anhydrous: 367.86 Hexahydrate: 475.94
Assay	Anhydrous: not less than 85.0% of $Na_5O_{10}P_3$ and not less than 56.0% and not more than 58.0% of P_2O_5 Hexahydrate: not less than 65.0% of $Na_5O_{10}P_3$ and not less than 43.0% and not more than 45.0% of P_2O_5
DESCRIPTION	White, slightly hygroscopic granules or powder
FUNCTIONAL USES	Sequestrant, texturizer
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Freely soluble in water; insoluble in ethanol
pH (FNP 5)	9.1 - 10.1 (1 % soln)
Test for phosphate (FNP 5)	Passes test
Test for sodium (FNP 5)	Passes test
PURITY	
Loss on drying (FNP 5)	Anhydrous: not more than 0.7% (105°, 1 h) Hexahydrate: not more than 23.5% (60°, 1 h, followed by 105°, 4 h)
Water-insoluble matter (FNP5)	Not more than 0.1%
Higher polyphosphates	Not detectable See description under TESTS

Fluoride (FNP 5)

Not more than 50 mg/kg (Method I or III)

Arsenic (FNP 5)

Not more than 3 mg/kg (Method II)

Lead

Not more than 4 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Higher polyphosphates

Chromatographic solvent: Mix 75 ml of isopropanol, 10 ml of water, 20 ml of 20% trichloroacetic acid and 0.3 ml of 20% ammonia. Make fresh every week.

Chromatographic spray: Dissolve 1 g of ammonium molybdate in 85 ml of water, 10 ml of N hydrochloric acid and 5 ml of 60% perchloric acid.

Sample solution: Dissolve 1 g of the sample in 50 ml of water.

Reference solution: Dissolve 1 g of a standard sample of pentasodium triphosphate in 50 ml of water.

Procedure: Place 0.01 ml of the sample solution and 0.01 ml of reference solution on the starting line of the chromatographic paper and allow to dry in a stream of warm air. Use ascending chromatography at 18-20° until the solvent has ascended about 25 cm from the starting line (12 - 15 h). Dry at 60° in an oven and spray with the chromatographic spray. Place the paper under an ultraviolet lamp and irradiate until the phosphates are visible as blue spots (about 2 min). Three spots (one from the monophosphate ($R_f = 0.69$), a second from the diphosphate ($R_f = 0.44$) and the third from the triphosphate ($R_f = 0.29$) are observed, and no other spot is observed.

METHOD OF ASSAY

1. Determination of $Na_5O_{10}P_3$

Reagents and solutions
- Potassium acetate buffer (pH 5.0): Dissolve 78.5 g of potassium acetate in 1000 ml of water and adjust the pH of the solution to 5.0 with acetic acid. Add a few mg of mercuric iodide to inhibit mould growth.
- 0.3 M Potassium chloride: Dissolve 22.35 g of potassium chloride in water, add 5 ml of potassium acetate buffer, dilute with water to 1000 ml, and mix. Add a few mg of mercuric iodide.
- 0.6 M Potassium chloride: Dissolve 44.7 g of potassium chloride in water, add 5 ml of potassium acetate buffer, dilute with water to 1000 ml, and mix. Add a few mg of mercuric iodide.
- 1 M Potassium chloride: Dissolve 74.5 g of potassium chloride in water, add 5 ml of potassium acetate buffer, dilute to 1000 ml with water, and mix. Add a few mg of mercuric iodide.

Chromatographic Column: Use a standard chromatographic column 20 to 40 cm length, 20 to 28 cm inside diameter, with a sealed-in, coarse porosity fritted disk. If a stopcock is not provided, attach a stopcock having a 3 to 4 mm, diameter bore to the outlet of the column with a short length of flexible vinyl tubing.

Procedure: Close the column stopcock, fill the space between the fritted disk and the stopcock with water, and connect a vacuum line to the stopcock. Prepare a 1:1 water slurry of Dowex F x 8, or equivalent, chloride form, 100-200 or 200-400 mesh, styrenedivinylbenzene ion exchange resin, and decant off any fine particles and any styrenedivinylbenzene ion exchange resin, and decant off any fine particles and any foam. Do this two or three times or until no more finely suspended material or foaming is observed. Fill the column with the slurry, and open the stopcock to allow the vacuum to pack the resin bed until the water level is slightly above the top of the resin, then immediately close the stopcock. Do not allow the liquid level to fall below the resin level at any time. Repeat this procedure until the packed resin column is 15 cm above the fritted disk. Place one circle of tightly fitting fibre filter paper on top of the resin bed, then place a perforated polyethylene disk on top of the paper. Alternatively, a loosely packed plug of glass wool may be placed on top of the bed. Close the top of the column with a rubber stopper in which a 7.6 cm length of capillary tubing (1.5 mm i.d., 7 mm o.d.) has been inserted through the centre, so that about 12 mm of the tubing extends through the bottom of the stopper. Connect the top of the capillary tubing to the stem of a 500-ml separator with flexible vinyl tubing, and clamp the separator to a ring stand above the column. Wash the column by adding 100 ml of water to the separator with all stopcocks closed. First open the separator stopcock, then open the column stopcock. The rate of flow should be about 5 ml per min. When the separator is empty, close the stopcock on the column then close the separator stopcock.

Transfer about 500 mg of the sample (a), accurately weighed, into a 250 ml volumetric flask, dissolve and dilute to volume with water, and mix. Transfer 10 ml of this solution into the separator, open both stopcocks and allow the solution to drain into the column, rinsing the separator with 20 ml of water. Discard the eluate. Add 370 ml of 0.3 M Potassium Chloride to the separator, and allow this solution to pass through the column, discarding the eluate. Add 250 ml of 0.6 M Potassium Chloride to the column, allow the solution to pass through the column, and receive the eluate in a 400-ml beaker. (To ensure a clean column for the next run, pass 100 ml of 1 M Potassium Chloride through the column, followed by 100 ml of water. Discard all washings.) To the beaker add 15 ml of nitric acid, mix, and boil for 15 to 20 min. Add methyl orange TS, and neutralize the solution with stronger ammonia TS. Add 1 g of ammonium nitrate crystals, stir to dissolve, and cool. Add 15 ml of ammonium molybdate TS, with stirring, and stir vigorously for 3 min or allow to stand with occasional stirring for 10 to 15 min. Filter the contents of the beaker with suction through a 6-7 mm paper pulp filter pad supported in a 25 mm porcelain disk. The filter pad should be covered with a suspension of a filtering aid. After the contents of the beaker have been transferred to the filter, wash the beaker with five 10 ml portions of a 1% solution of sodium or potassium nitrate, passing the washings through the filter, then wash the filter with five 5-ml portions of the wash solution. Return the filter pad and the precipitate to the beaker, wash the funnel thoroughly with water into the beaker, and dilute to about 150 ml. Add 0.1 N sodium hydroxide from a buret until the yellow precipitate is dissolved, then add 5 to 8 ml in excess. Add phenolphthalein TS, and titrate the excess alkali with 0.1 N nitric acid. Finally, titrate with 0.1 N sodium hydroxide to the first appearance of the pink colour. The difference between the total volume of 0.1 N sodium hydroxide added and the volume of nitric acid required represents the volume, V, in ml, of 0.1 N sodium hydroxide consumed by the phosphomolybdate complex.

Calculate the $Na_5O_{10}P_3$ content of the sample in % by the formula:

$$\% Na_5 O_{10} P_3 = \frac{0.533 \times 25 \times V}{a} \times 100$$

where

a = the weight of the sample (mg)

2. Determination of P_2O_5

Accurately weigh about 20 g of the sample into a beaker. Add 150 ml water and 20 ml concentrated nitric acid. Introduce anti-bumping granules, cover the beaker with a watch glass and boil gently for 1 h. Cool to room temperature. Quantitatively transfer the solution to a 500-ml volumetric flask, dilute with water, mix well and dilute to the mark with water. Transfer 20.0 ml of the solution to a plastic beaker, dilute to about 50 ml with water and place the beaker in an automatic titrator equipped with a pH meter. Adjust the pH of the solution to between 2.5 and 2.8 with 5 mol/l sodium hydroxide. Titrate the solution with 0.5 mol/l sodium hydroxide. Record the consumed volumes at the inflection points at about pH 4 (V1) and about pH 9 (V2).

Calculate the P_2O_5 content of the sample in % by the formula:

$$\% \ P_2O_5 = [(V2 - V1)/2000] \times f \times 70.97 \times (500/20) \times (100/w)$$

$$= [(V2 - V1)/w] \times f \times 88.71$$

where
w = weight of the sample (g)
f = factor of 0.5 mol/l sodium hydroxide (= actual molarity/0.5)

PROTEASE FROM *ASPERGILLUS ORYZAE*, VAR.

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Acceptable" was established at the 31st JECFA (1987).

SYNONYMS	INS No.1101(i)
SOURCES	Produced by the controlled fermentation of non-toxicogenic and non-pathogenic strains of *Aspergillus oryzae* and isolated from the growth medium.
ACTIVE PRINCIPLES	Endo- and exopeptidases
SYSTEMATIC NAMES AND NUMBERS	1. Aminopeptidases (EC 3.4.11) 2. Serine endopeptidases (EC 3.4.21) 3. Aspartic endopeptidases (EC 3.4.23)
REACTIONS CATALYZED	1. Hydrolysis of proteins at the N-terminal, liberating amino acids 2. Hydrolysis of proteins containing serine peptide bonds 3. Hydrolysis of proteins containing aspartic acid bonds
SECONDARY ENZYME ACTIVITIES	α-Amylase (EC 3.2.1.1)
DESCRIPTION	Off-white to tan amorphous powders dispersed in food-grade diluents or carriers; may contain stabilizers and preservatives; soluble in water and practically insoluble in ethanol and ether
FUNCTIONAL USES	Enzyme preparation Used in the preparation of and/or in meat and fish products, beverages, soup and broths, dairy and bakery products
GENERAL SPECIFICATIONS	Must conform to the General Specifications for Enzyme Preparations Used in Food Processing (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7)
CHARACTERISTICS	
IDENTIFICATION	
Proteolytic activity (FNP 5)	The sample shows proteolytic activity; use method Proteolytic activity, Fungal (HUT)

QUILLAIA EXTRACTS

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 29th JECFA (1985) and published in FNP 34 (1986) and in FNP 52 (1992). An ADI of 0-5mg/kg bw was established at the 29th JECFA (1985).

SYNONYMS	Quillaja extracts, Soapbark extracts, Quillay bark extracts, Bois de Panama, Panama bark extracts, Quillai extracts; INS No. 999
DEFINITION	Obtained by aqueous extraction of the milled inner bark of *Quillaja saponaria* Molina (family *Rosaceae*) or of the wood, including stems and branches. Quillaia extracts (QE) contain a number of triterpenoid saponins (QS) consisting of glycosides of quillaic acid, some sugars (including glucose, galactose, arabinose, xylose and rhamnose) along with polyphenols (including tannins), calcium oxalate and other minor components. The QS contains sugars linked to the triterpene at carbon 3 (glucuronic acid and two of the following three sugars: galactose, rhamnose or xylose) and at carbon 28 (rhamnose, fucose, xylose, glucose and arabinose). The principal saponin component of commercial QE is designated as QS-18. Quillaia extracts are available commercially as "non-refined" and "semi-refined" extracts, each of which may be sold as aqueous solutions or as dried powders. The extracts are usually preserved with sodium benzoate or ethanol. Fresh non-refined QE contains an average value of 190 g of QS/kg. ("Highly refined" quillaia extract, which is not specified by this monograph, is typically used in human and animal vaccines)
Formula weight	Monomeric saponins from about 1800 up to about 2000
Assay	QS as specified by the vendor.
DESCRIPTION	Non-refined liquid extract has a red-brownish colour; the powder form is light brown with a pink tinge. The liquid or powder semi-refined QE has a light colour.
FUNCTIONAL USES	Emulsifier, foaming agent.
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Very soluble in water, insoluble in ethanol, acetone, methanol and butanol
Foam	Dissolve 0.5 g in 9.5 g of water. Add 1 ml of this mixture to 350 ml of water in a 1000 ml graduated cylinder. Cover the cylinder and vigorously shake 30 times and allow to settle. Record the foam level in ml after 30 min. Typical values are 150 ml of foam.
QS-18 saponin	Determine as in Method of Assay. The major peak of the sample is compared to the QS-18 peak of the standard.
Colour and Turbidity	Powdered form only: Dissolve 0.5 g in 9.5 g of water. The solution must be free of any visible aggregates. Determine the solution absorbance against water, at 520 nm. Maximum acceptable levels are 1.2 absorbance units.
PURITY	
Water (FNP 5)	Powdered form: not more than 6% (Karl Fischer Method)
Loss on drying (FNP 5)	Liquid form: 50 to 70% (2g, 105°, 5 h).

pH (FNP 5)

4.2 - 5.5 (4 % solution).

Ash (FNP 5)

Not more than 12% on dry basis (use 1.0 g of the powder-form sample; for liquid sample use residue from loss on drying).

Tannins

Not more than 7 % on dry basis.
See description under TESTS

Lead

Not more 2 mg/kg.
Determine using atomic absorption technique appropriate to the specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Tannins

Weigh 3 g of the powder form or equivalent amount of liquid sample, based on solids content determined from loss on drying. Dissolve in 250 ml of water. Adjust the pH to 3.5 with acetic acid. Dry 25 ml of this solution at 105 ° for 5h to determine the dry weight in g solids/l (S initial). 50 ml of the solution are mixed with 360 mg of polyvinyl polypyrrolidone (PVPP). Stir the solution for 30 min at room temperature, followed by centrifugation at 3000 rpm. Recover the supernatant and determine dry weight after drying at 105 °, 5 h (S final). The amount of tannins in the sample is estimated as:

% tannins on dry basis= 100 x (S initial – S final) / S initial

S initial: g solids / l before treatment with PVPP
S final: g solids / l after treatment with PVPP

METHOD OF ASSAY

Sample Preparation:
For powder sample dissolve 0.5 g in 9.5 g of water and filter through 0.2 µm filter before injection, into HPLC. For aqueous extracts (~ 550 g solids/l) dilute 1 g in 9 g of water and filter through 0.2 µm filter before injection.

Standard preparation:
Dissolve 1.5 g of purified saponins (SuperSap, Natural Response, Chile; Quil-A, Superfos., Denmark or similar, contain at least 90% saponin by weight) in 100 ml of water and filter through 0.2 micron filter before injection.
Reverse phase HPLC conditions:

Column: Vydac 214TP54 or similar, 4.6 x 250 mm length, 5µm pore
Column temperature: room temperature
Pump: Linear gradient
A: 0.15% TFA in HPLC grade water.
B: 0.15% TFA in HPLC grade acetonitrile.

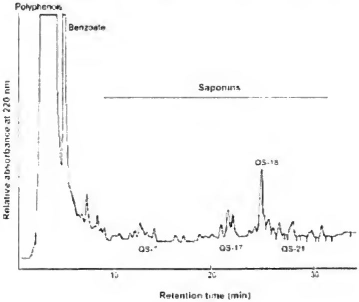
Gradient	Time(min)	% solvent A	% solvent B
	0	70	30
	40	55	45
	45	70	30

Flow rate: 1 ml/min
Injection volume: 20 µl

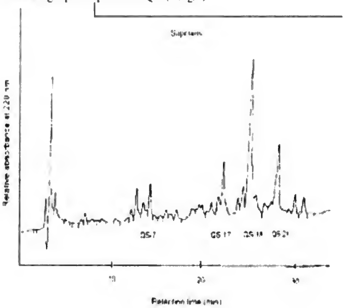
Calculation:
Compare the area of saponins in the sample to that of the standard. Estimate the concentration of QS in g/l as

QS (g/l)= (Asample/Astandard) (13.5 g / l)

Where 13.5 g/l corresponds to the concentration of the standard injected (15 g/l, Example: Chromatograph of non-refined QE (55 g solids/l). The peak labeled QS-18 is the dominant saponin in QE extract.



Chromatograph of purified QS (15 g/l)



RENNET FROM *RHIZOMUCOR* SPECIES

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 15th JECFA (1971) and published in NMRS 50B (1972) and in FNP 52 (1992). An ADI "Not specified" was established at the 18th JECFA (1974).

SOURCES	Produced by the controlled fermentation of non-pathogenic and non-toxicogenic strains of *Rhizomucor miehei* or *Rhizomucor pusillus.*
ACTIVE PRINCIPLE	Microbial aspartic proteinase (acid protease)
SYSTEMATIC NAME AND NUMBER	EC 3.4.23.23; C.A.S. No. 9073-79-4
REACTIONS CATALYZED	Hydrolyzes polypeptides, e.g. casein, yielding peptides of lower molecular weight.
DESCRIPTION	White to tan amorphous powders; soluble in water, the solution usually being light yellow in colour; practically insoluble in ethanol and ether.
FUNCTIONAL USES	Enzyme preparation Used in clotting of milk for cheese production
GENERAL SPECIFICATIONS	Must conform to the "General Specifications for Enzyme Preparations Used in Food Processing" (FNP 52 as amended in FNP 52 Add 6 and FNP 52 Add 7)
CHARACTERISTICS	
IDENTIFICATION	
Milk clotting activity (FNP 5)	The sample shows milk clotting activity

SHELLAC, BLEACHED

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 51st JECFA (1998) and published in FNP 52 Add 6 (1998). An ADI "Acceptable, present uses (as a coating, glazing, and surface-finishing agent externally applied to food) not of toxicological concern" was established at the 39th JECFA (1992).

SYNONYMS INS No. 904

DEFINITION Shellac is a polyester resin obtained from lac, the resinous secretion of the insect *Laccifer (Tachardia) lacca* Kerr (Fam. *Coccidae*). Bleached shellac is obtained by dissolving the lac in aqueous sodium carbonate, followed by bleaching with sodium hypochlorite, precipitation of the bleached lac with dilute sulfuric acid solution, and drying; wax-free bleached shellac is prepared by further treatment whereby the wax is removed by filtration.

C.A.S. number 9000-59-3

DESCRIPTION Bleached shellac: off-white to tan, amorphous granular resin; wax-free bleached shellac: light yellow, amorphous, granular resin

FUNCTIONAL USES Coating agent, glazing agent, surface finishing agent

CHARACTERISTICS

IDENTIFICATION

Colour reaction To 50 mg of the sample add a few drops of a solution of 1 g ammonium molybdate in 3 ml of sulfuric acid. A green colour is produced, changing to lilac when the solution is neutralized with 6 N ammonium hydroxide.

Solubility (FNP 5) Insoluble in water; freely (though very slowly) soluble in ethanol; slightly soluble in acetone and ether

Acid value Between 60 and 89
See description under TESTS

PURITY

Loss on drying (FNP 5) Not more than 6% (40°, 4 h, then room temperature over silica gel, 15 h)

Rosin Dissolve 2 g of the sample in 10 ml of dehydrated ethanol, and add slowly, with shaking, 50 ml of solvent hexane. Transfer to a separator, wash with two 50-ml portions of water, and discard the washings. Filter the solvent layer, evaporate it to dryness, and to the residue add 2 ml of a mixture of 1 volume of liquefied phenol and 2 volumes of methylene chloride. Stir and transfer a portion of the mixture to a cavity of a colour-reaction plate. Fill an adjacent cavity with a mixture of 1 volume of bromine and four volumes of methylene chloride, and cover both cavities with an inverted watch glass. No purple or deep indigo blue colour is produced in or above the liquid containing the sample residue.

Wax Bleached shellac: not more than 5.5%; wax-free bleached shellac, not more than 0.2%
See description under TESTS

Lead Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

TESTS

IDENTIFICATION TESTS

Acid value

Dissolve about 1 g of finely ground sample, accurately weighed, in 50 ml of alcohol previously neutralized to phenolphthalein with sodium hydroxide, and titrate with 0.1 N potassium hydroxide. Determine the end point using phenolphthalein TS or a potentiometer. If phenolphthalein is used, titrate until the pink colour persists for at least 30 sec. Calculate the acid value by the formula 56.1V x N/W, in which V is the exact volume, in ml, N is the exact normality of the sodium hydroxide solution, and W is the weight, in g, of sample taken, calculated on the dry basis.

PURITY TESTS

Wax

Transfer about 10 g of finely ground sample, accurately weighed, and 2.5 g of sodium carbonate to a 200-ml tall-form beaker. Add 150 ml of hot water, immerse the beaker in a boiling water bath, and stir until the sample is dissolved. Cover the beaker with a watch glass, heat for 3 h without agitation, and cool in a cold water bath. When the wax has floated to the surface, filter the mixture through medium-speed quantitative ashless filter paper, transferring the wax to the paper, and wash the filter with water. Pour 5 to 10 ml of ethanol onto the filter to accelerate drying. Wrap the paper loosely in a large piece of filter paper, bind with a piece of fine wire, and dry with the aid of gentle heat. Extract with chloroform in a suitable continuous extraction apparatus for 2 h, using a previously dried and accurately weighed flask to receive the extracted wax and solvent. Evaporate the solvent, dry the wax at 105° to constant weight, and calculate the percentage of wax.

SMOKE FLAVOURINGS
(Tentative)

Prepared at the 55th JECFA (2000) and published in FNP 52 Add. 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). An ADI "Provisional acceptance" was established at the 31st JECFA (1987).

Information required on: alternative solvent to benzene in the method of analysis for carbonyls (proposals should be supported by a comparative test of the method with benzene and the proposed alternative); comments on other sections of the monograph are also invited.

SYNONYMS Wood smoke flavour, Smoke condensates

DEFINITION Complex mixtures of components of smoke obtained by subjecting untreated hardwoods to (a) pyrolysis in a limited and controlled amount of air, (b) dry distillation between 200° and 800°, or (c) superheated steam between 300° and 500°. Source materials must not contain detectable amounts of pesticides, wood preservatives, or other extraneous matter that may result in hazardous constituents in the wood smoke. The major flavouring principles of Smoke Flavourings are carboxylic acids, compounds with carbonyl groups and phenolic compounds.

During manufacture, wood smoke is subjected to an aqueous extraction system or to distillation, condensation, and separation for collection of the aqueous phase, which serves to remove hazardous constituents, such as polycyclic aromatic hydrocarbons. The aqueous smoke fraction containing water-soluble constituents may be diluted with water or be extracted with an edible vegetable oil to produce a smoke flavouring with higher levels of non-polar constituents that may be further extracted using food grade substances, such as propylene glycol or aqueous solutions of polysorbates.

Commercial products may also contain additives such as emulsifiers, antifoaming agents, and gums. Smoke flavourings may also be prepared in dry form with the addition of carriers, such as yeasts, flours, salt, phosphates, carbohydrates, and anti-caking agents.

These specifications apply only to the water-soluble distillates of condensed wood smoke, their aqueous/vegetable oil or polysorbate extracts and concentrates of these, and not to products derived from the water-insoluble tars. These specifications do not apply to commercial products, as described in the previous paragraph, nor to pyroligneous acid, a by-product of the manufacture of charcoal by carbonation of wood in the absence of air.

Assay
Acidity: 2 to 20% (as acetic acid)
Carbonyls: 2 to 25% (as heptaldehyde)
Phenols: 0.1 to 16% (as 2,6-dimethoxyphenol)

DESCRIPTION Light brown to dark amber liquids; smoky odour

FUNCTIONAL USES Flavouring agent, colour

CHARACTERISTICS

IDENTIFICATION Characteristic appearance and odour

PURITY

Benzo(a)pyrene
Not more than 2 µg/kg
See description under TESTS

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods."

TESTS

PURITY TESTS

Benzo(a)pyrene

Caution: Benzo(a)pyrene and other polycyclic aromatic hydrocarbons are known carcinogens. The analyst must exercise appropriate care in handling them.

Principle: Benzo(a)pyrene (BaP) is one of several polycyclic aromatic hydrocarbons (PAHs) that may occur in liquid smoke flavourings. Its quantitation is used as an indicator for levels of PAHs in liquid smoke flavourings. BaP, as well as other PAHs are isolated from the sample by digestion and liquid extraction, and purified by solid phase extraction. Quantitation is accomplished by high performance liquid chromatography with fluorescence detection (FNP 5).

Apparatus:
- Liquid chromatograph with fluorescence detector and reverse-phase column, such as Vydac 201TP54, 4.6 x 250 mm, thermostated at 30E
- Digestion apparatus consisting of 250 ml round-bottom flask, 250 ml heating mantle, reflux condenser, and variable transformer
- Rotary evaporator, equipped with water bath set at 40E
- Pear-shaped flasks, 50 ml and 100 ml
- 30 ml Buchner funnels with coarse-porosity fritted disks
- Silica solid phase extraction (SPE) column, 6 ml capacity, 1000 mg packing, such as Bakerbond
- C_{18} SPE column, 6 ml capacity, 1000 mg packing, such as Bakerbond
- Stopcocks with Luer fitting (for SPE columns)
- PTFE syringe filter units, 13 mm diam., 0.45 micrometer porosity

Reagents:
- UV- or HPLC-grade hexane, methylene chloride, acetonitrile, and water
- Anhydrous ethanol, distilled before use
- Sodium sulfate, anhydrous, granular

Solutions:
- 0.8 g/ml aqueous potassium hydroxide
- Commercial PAH Standard Solution in acetonitrile, such as NIST Standard Reference Material 1647 (National Institute of Standards and Technology, Gaithersburg, MD 20899, USA)
- PAH working standards: prepare at least 4 working standards in 50% acetonitrile/50% water (in the range of 0.5 to 10 µg/l) from the commercial PAH Standard Solution.

Procedure: *Caution*: Due to the toxicity of solvents used in this method, the use of gloves is recommended.

SAMPLE PREPARATION
Weigh 10 g of liquid smoke flavouring into a 250 ml round-bottom flask. Add 20 ml ethanol, 2 ml 0.8 g/ml aqueous KOH solution, and a few boiling chips. Assemble the digestion apparatus, set the variable transformer to 50% output, and reflux the sample for 2 hr. Let cool about 15 min. Transfer the digest to a 250 ml separatory funnel; rinse the flask with 20 ml water, 10 ml ethanol, and 15 ml hexane and add to the separatory funnel; extract by shaking gently for 2 min. Drain the lower layer into a second separatory funnel and repeat the extraction with 15 ml hexane. Discard the lower layer. To each retained hexane layer add about 3 ml water and swirl. Discard

the water washes. Pass each hexane layer through a Buchner funnel containing 25 g sodium sulfate (pre-washed with 15 ml hexane) into a 100 ml pear-shaped flask. Rinse the sodium sulfate with 15 ml hexane; apply gentle pressure to the top of the funnel with heel of hand to force residual solvent through the sodium sulfate. Concentrate to about 1 ml on a rotary evaporator. Attach a stopcock to the outlet of the silica SPE column and condition the column with 15 ml methylene chloride, followed by 3 ml hexane; close the stopcock. (If there is a delay between column conditioning and charging the column with the sample, close the stopcock, leaving about 1 mm hexane above the head of the column. Just before loading the sample extract onto the column, open the stopcock to drain the excess solvent; then, close the stopcock.) Transfer the concentrated sample extract from the pear-shaped flask to the column, using two 1 ml portions of hexane to rinse. Open the stopcock and allow the sample to pass onto the column using gravity flow only, discarding the eluate. Elute the sample (by gravity) with 5 ml of 25% methylene chloride/75% hexane, discarding the first milliliter; collect the eluate in a 50 ml pear-shaped flask. Use pressure from a syringe to force residual solvent through the column. Add 4 ml acetonitrile and concentrate the sample extract to < 1 ml on a rotary evaporator.

Attach a stopcock to the outlet of the C_{18} column and condition it with 15 ml methylene chloride, followed by 5 ml acetonitrile. Close the stopcock. Transfer the concentrated sample extract to the column using two 0.5 ml portions of acetonitrile to rinse the flask. Open the stopcock to charge the column with the sample; discard the eluate. Elute the sample with 5 ml of 10% methylene chloride/90% acetonitrile, collecting the eluate in a 50 ml pear-shaped flask. Use a syringe to force residual solvent through the column. Concentrate the eluate to < 1 ml on a rotary evaporator. Transfer to a 5 ml volumetric flask, using three 0.5 ml portions of acetonitrile to rinse. Add 2.5 ml water, and dilute to 5.0 ml with acetonitrile. Filter through a PTFE syringe filter.

HIGH PERFORMANCE LIQUID CHROMATOGRAPHY
Analyse the filtered sample extract and the PAH working standards for BaP.
Chromatographic conditions:

- Solvent flow rate: 1.0 ml/min
- Solvent program: 3 min hold at 50% acetonitrile/50% water; linear gradient to 100% acetonitrile in 15 min; and 8 min hold at 100% acetonitrile
- fluorescence detector: excitation wavelength - 290 nm; emission wavelength - 410 nm
- Injection volume: 100 µl

The retention time of BaP is approximately 24 min. Using the peak heights for BaP in the standards, prepare a calibration curve of peak height vs. concentration (µg/l), and determine the slope (S) and the intercept (I). Calculate the concentration of BaP:

$$\text{BaP } (\mu g/kg) = V(H-I)/(S \times W)$$

where
H = the peak height of BaP in the sample extract
W = the weight of the sample (10 g)
V = the volume of the filtered sample extract (5.0 ml).

METHOD OF ASSAY

Acidity

Accurately weigh about 1 ml of sample in a 250 ml beaker. Dilute with about 100 ml of water. Titrate with 0.1 N sodium hydroxide solution to an equivalence point of pH 8.15, as determined using a by pH meter. Calculate acidity as percent by weight of acetic acid using the factor: 1 ml of 0.1 N sodium hydroxide is equivalent to 60.05 mg acetic acid.

Carbonyls

Principle: The total carbonyls of Smoke Flavourings are determined spectrophotometrically by reaction with 2,4-dinitrophenylhydrazine (2,4-DNPH) and expressed as heptaldehyde. The carbonyls of liquid smoke are converted to hydrazone derivatives by reaction with 2,4-DNPH in acid medium at 60°. A red pigment is formed on adjusting to alkaline pH and the absorbance is read at 430 nm.

Apparatus: Spectrophotometer with 1 cm cuvettes, water bath at 60±5°, 25 ml volumetric flasks, miscellaneous glassware.

Reagents:
- Benzene
- Ethanol (anhydrous): Render carbonyl-free by adding 1% 2,4-DNPH, a few drops of concentrated HCl, refluxing 3 h and distilling.
- 2,4-DNHP: Recrystallize from carbonyl-free methanol.
- Potassium hydroxide pellets (KOH)
- Heptaldehyde
- Trichloroacetic Acid (TCA)

Solutions:
(1) Saturated 2,4 -DNPH: 0.05% in benzene. Shake for 1 h or prepare 1 day in advance and allow to settle overnight. Insoluble crystals of 2,4-DNPH should be present. Filter the upper layer prior to use. Prepare fresh weekly.
(2) KOH solution: 4% w/v in carbonyl-free ethanol. Prepare fresh daily.
(3) TCA solution: 4% w/v in benzene. Stable at room temperature.
(4) 0.1% Smoke Flavouring, prepared as follows: 1 ml or 1 gram sample dissolved or diluted to 50 ml with carbonyl-free alcohol of which 5 ml is diluted to 100 ml with a 10% carbonyl-free ethanol - 90% benzene solution.
(5) Heptaldehyde standard solution: 30 μg/ml in benzene.

Procedure: Place 1 ml of diluted sample (Solution 4) in a 15 ml volumetric flask and 1 ml benzene in another flask to serve as the blank.

Add to each volumetric flask:
- 1 ml benzene
- 2 ml saturated 2,4-DNPH solution (Solution 1)
- 2 ml TCA solution (Solution 3)

Cover with glass stoppers and heat for 30 min at 60°. Immediately cool in an ice bath. Add 5 ml of KOH solution (Solution 2) and dilute to 25 ml with carbonyl-free ethanol. Allow colour to develop exactly 10 min after addition of Solution 2, then read absorbance at 430 nm. Correct absorbance for the blank.

Construct a calibration curve using the standard Heptaldehyde solution (solution 5) in the range of 1-30 μg/ml plotting absorbance at 430 nm versus concentration.

Calculate % Carbonyls (as heptaldehyde) from the calibration curve, correcting for dilution of the sample.

Phenols

Principle: Phenolic compounds can be determined spectrophotometrically after reacting with 2,6-Dibromo-N-chloro-p-benzoquinoneimine (BQC) in a basic buffer. The method cannot differentiate between phenolic compounds but gives reproducible results expressed as 2,6-dimethoxyphenol (2,6-DMP). A solution of sample is reacted with BQC reagent in a basic borate buffer to form indophenols, which have a blue colour. The colour developed is quantitated at 610 nm using a standard curve prepared with 2,6-DMP.

Apparatus:
- Spectrophotometer with 1 cm cells
- 100 ml volumetric flasks
- Centrifuge
- Assorted glassware

Reagents:
- Cupric sulfate ($CuS0_4 \cdot 5H_20$)
- Sodium borate ($Na_2B_40_7 \cdot 10H_20$)
- Sodium hydroxide
- 2,6-Dibromo-N-chloro-p-benzoquinoneimine
- 2,6-Dimethoxyphenol
- 1-Butanol
- Methanol

Solutions:
(1) 0.05% w/v $CuSO_4 \cdot 5H_2O$ in water.
(2) 24.8 g $Na_2B_40_7 \cdot 10H_2O$ dissolved in 900 ml water. Adjust pH to 9.8 with sodium hydroxide TS and add water to 1,000 ml volume.
(3) 40 mg BQC dissolved in 10 ml methanol. (Prepare fresh daily.)
(4) 2,6-Dimethoxyphenol in water, 20 μg/ml.
(5) 0.2% Smoke Flavourings in water.

Procedure: Place 5 ml of diluted sample solution (Solution 5) in one test tube and 5 ml of water in another test tube to serve as the blank. Then add to each tube:
- 1 ml of cupric sulfate solution (Solution 1).
- 5 ml of borate buffer (Solution 2).
- 4 drops of BQC reagent (Solution 3).

Cover each tube, shake vigorously, and allow colour development in the dark for exactly 10 min. Add 10 ml of 1-butanol to each test tube, cover and invert 6 to 8 times (do not shake). Centrifuge test tubes for 5 min at 700 rpm.

Measure the absorbance of the sample at 610 nm and correct for the blank. Construct a calibration curve using the standard 2,6-DMP solution (Solution 4) in the range of 1-20 μg/ml, plotting absorbance at 610 nm versus concentration.

Calculate percent Phenols Content (as 2,6-DMP) from the calibration curve, correcting for dilution of the sample.

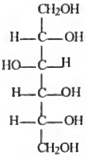
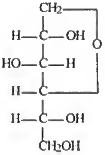
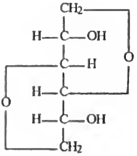
SODIUM SULFATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 53rd JECFA (1999) and published in FNP 52 Add 7 (1999). A temporary ADI "Not specified" was established at the 53rd JECFA (1999).

SYNONYMS	Glauber's salt (decahydrate form); INS No. 514
DEFINITION	
C.A.S. number	7757-82-6 (Anhydrous) 7727-73-3 (Decahydrate)
Chemical formula	$Na_2SO_4 \cdot xH_2O$ (x = 0 or 10)
Formula weight	142.04 (Anhydrous) 322.19 (Decahydrate)
Assay	Not less than 99.0 % on the dry basis
DESCRIPTION	Colourless crystals or fine, white crystalline powder. The decahydrate is efflorescent.
FUNCTIONAL USES	Colour adjuvant
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Freely soluble in water; practically insoluble in ethanol
Test for sodium (FNP 5)	Passes test
Test for sulfate (FNP 5)	Passes test
PURITY	
Loss on drying (FNP 5)	Anhydrous: Not more than 1% (105°, 4 h) Decahydrate: Between 51.0% and 57.0% (105°, 4h)
Selenium (FNP 5)	Not more than 30 mg/kg Test 0.2 g of the sample as directed in the Limit Test (Method II)
Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation, may be based on the principles of the method described in FNP 5, " Instrumental Methods".
METHOD OF ASSAY	Weigh accurately about 0.5 g of the dried sample, dissolve in 200 ml of water, add 1 ml of hydrochloric acid and heat to boiling. Gradually add, in small portions and while stirring constantly, an excess of hot barium chloride TS (about 10 ml), and heat the mixture on a steam bath for 1 h. Collect the precipitate on a filter, wash until free from chloride, dry, ignite and weigh. The weight of the barium sulfate so obtained, multiplied by 0.6086 corresponds to the equivalent amount of Na_2SO_4.

SORBITAN MONOLAURATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 44th JECFA (1995) and published in FNP 52 Add 3 (1995). A group ADI of 0-25 mg/kg bw for sorbitan esters of lauric, oleic, palmitic, and stearic acid was established at the 26th JECFA (1982).

SYNONYMS	Sorbitan laurate; INS No. 493
DEFINITION	A mixture of the partial esters of sorbitol and its mono- and dianhydrides with edible lauric acid
C.A.S. number	1338-39-2
Structural formula	Contains lauric acid esterified with polyols derived from sorbitol including the following types:  Sorbitol  1,4-Sorbitan  Isosorbide
Assay	Saponification of 100 g of the sample yields not less than 36 g and not more than 49 g of polyols, and not less than 56 g and not more than 68 g of fatty acids. The polyol content shall be not less than 95% of a mixture of sorbitol, 1,4-sorbitan and isosorbide.
DESCRIPTION	Amber-coloured oily viscous liquid, light cream to tan beads or flakes or a hard, waxy solid with a slight odour
FUNCTIONAL USES	Emulsifier, stabilizer
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Dispersible in hot and cold water
PURITY	
Water (FNP 5)	Not more than 2% (Karl Fischer Method)
Sulfated ash (FNP 5)	Not more than 0.5%
Acid value (FNP 5)	Not more than 7
Saponification value (FNP 5)	Not less than 155 and not more than 170
Hydroxyl value (FNP 5)	Not less than 330 and not more than 358

Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods"

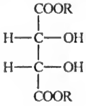
METHOD OF ASSAY

Transfer about 25 g of the sample, accurately weighed, into a 500-ml round-bottom flask, add 250 ml of alcohol and 7.5 g of potassium hydroxide, and mix. Connect a suitable condenser to the flask, reflux the mixture for 1 to 2 h, and then transfer to an 800-ml beaker, rinsing the flask with about 100 ml of water and adding it to the beaker. Heat on a steam bath to evaporate the alcohol, adding water occasionally to replace the alcohol, and evaporate until the odor of alcohol can no longer be detected. Adjust the final volume to about 250 ml with hot water. Neutralize the soap solution with dilute sulfuric acid (1 in 2), add 10% in excess, and heat, while stirring, until the fatty acid layer separates. Transfer the fatty acids to a 500-ml separator, wash with three or four 20-ml portions of hot water to remove polyols, and combine the washings with the original aqueous polyol layer from the saponification. Extract the combined aqueous layer with three 20-ml portions of petroleum ether, add the extracts to the fatty acid layer, evaporate to dryness in a tared dish, cool and weigh.

Neutralize the polyol solution with a 1 in 10 solution of potassium hydroxide to pH 7 using a suitable pH meter. Evaporate this solution to a moist residue, and separate the polyols from the salts by several extractions with hot alcohol. Evaporate the alcohol extracts on a steam bath to dryness in a tared dish, cool, and weigh. Avoid excessive drying and heating.

STEARYL TARTRATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 46th JECFA (1996) and published in FNP 52 Add 4 (1996). No ADI was established, but a level of use of 0 - 500 mg/kg in flour was accepted at the 9th JECFA (1965).

SYNONYMS	Stearyl palmityl tartrate; INS No. 483
DEFINITION	The product of the esterification of tartaric acid with commercial stearyl alcohol, which consists essentially of stearyl and palmityl alcohols; consists mainly of diester, with minor amounts of monoester and of unchanged starting materials
Chemical names	Main components are distearyl tartrate, dipalmityl tartrate and stearylpalmityl tartrate
Chemical formula	Distearyl tartrate: $C_{40}H_{78}O_6$ Dipalmityl tartrate: $C_{36}H_{70}O_6$ Stearylpalmityl tartrate: $C_{38}H_{74}O_6$
Structural formula	 Where R = $(CH_2)_{17}CH_3$ or $(CH_2)_{15}CH_3$
Formula weight	Distearyl tartrate: 655.06 Dipalmityl tartrate: 598.95 Stearylpalmityl tartrate: 627.00
Assay	Not less than 90% of total ester content corresponding to an ester value within the range of 163 to 180
DESCRIPTION	Cream-coloured unctuous substance
FUNCTIONAL USES	Flour treatment agent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, insoluble in cold ethanol, soluble in hot ethanol
Melting range (FNP 5)	67 - 77°
Hydroxyl value (FNP 5)	200 to 220
Test for tartrate (FNP 5)	Passes test
PURITY	
Sulfated ash (FNP 5)	Not more than 0.5% Test 2 g of the sample (Method I)
Total tartaric acid	Not less than 18% and not more than 35% See description under TESTS

Unsaponifiable matter

Not less than 77% and not more than 83%
See description under TESTS

Acid value

Not more than 6
See description under TESTS

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparations may be based on the principles of method described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Total tartaric acid

Standard Curve
Transfer 100 mg of reagent-grade tartaric acid, accurately weighed, into a 100-ml volumetric flask, dissolve it in about 90 ml of water, add water to volume, and mix well. Transfer 3.0-, 4.0-, 5.0-, and 6.0-ml portions into separate 19 x 150-mm matched cuvettes, and add sufficient water to make 10.0 ml. To each cuvette add 4.0 ml of a freshly prepared 1 in 20 solution of sodium metavanadate and 1.0 ml of acetic acid. (Note: Use these solutions within 10 min after color development.) Prepare a blank in the same manner, using 10 ml of water in place of the tartaric acid solutions. Set the instrument at zero with the blank, and then determine the absorbance of the four solutions of tartaric acid at 520 nm with a suitable spectrophotometer or a photoelectric colorimeter equipped with a 520-nm filter. From the data thus obtained, prepare a standard curve by plotting the absorbances on the ordinate against the corresponding quantities, in mg, of the tartaric acid on the abscissa.

Test Preparation
Transfer about 4 g of the sample, accurately weighed, into a 250-ml Erlenmeyer flask, and add 80 ml of approximately 0.5N potassium hydroxide and 0.5 ml of phenolphthalein TS. Connect an air condenser at least 65 cm in length to the flask, and heat the mixture on a hot plate for about 2.5 h. Add to the hot mixture approximately 10% phosphoric acid until it is definitely acid to congo red test paper. Reconnect the air condenser, and heat until the fatty acids are liquified and clear. Cool and then transfer the mixture into a 250-ml separator with the aid of small portions of water and chloroform. Extract the liberated fatty acids with three successive 25-ml portions of water, and add the washings to the separator containing the water layer. Transfer the contents of the first separator to a 250-ml beaker, heat on a steam bath to remove traces of chloroform, filter through acid-washed, fine-texture filter paper into a 500-ml volumetric flask, and finally dilute to volume with water (Solution I). Pipet 25.0 ml of this solution into a 100-ml volumetric flask, and dilute to volume with water (Solution II).

Procedure
Transfer 10.0 ml of Solution II prepared under Test Preparation into a 19 x 150-mm cuvette. Add 4.0 ml of a freshly prepared 1 in 20 solution of sodium metavanadate and 1.0 ml of acetic acid. (Note: Use these solutions within 10 min after color development.) Prepare a blank in the same manner, using 10 ml of water in place of the tartaric acid solutions. Set the instrument at zero with the blank, and then determine the absorbance of the solution at 520 nm with a suitable spectrophotometer or a photoelectric colorimeter equipped with a 520-nm filter. From the standard curve determine the weight, in mg, of tartaric acid in the final dilution, multiply this by 20, and divide the result by the weight of the original sample to obtain the percentage of tartaric acid.

Unsaponifiable matter

This procedure determines those substances frequently found dissolved in fatty materials that cannot be saponified by alkali hydroxides but that are soluble in ordinary fat solvents.

Procedure

Weigh accurately 5.0 g of the sample into a 250-ml flask, add a solution of 2 g potassium hydroxide in 40 ml of alcohol, and boil gently under a reflux condenser for 1 h. Transfer the contents of the flask to a glass-stoppered extraction cylinder (approximately 30 cm in length, 3.5 cm in diameter, and graduated at 40, 80, and 130 ml). Wash the flask with sufficient alcohol to make a volume of 40 ml in the cylinder, and complete the transfer with warm and then cold water until the total volume is 80 ml. Finally, wash the flask with a few ml of petroleum ether, add the washings to the cylinder, cool the contents of the cylinder to room temperature, and add 50 ml of petroleum ether.

Insert the stopper, shake the cylinder vigorously for at least 1 min, and allow both layers to become clear. Siphon the upper layer as completely as possible without removing any of the lower layer, collecting the ether fraction in a 500-ml separator. Repeat the extraction and siphoning at least six times with 50-ml portions of petroleum ether, shaking vigorously each time. Wash the combined extracts, with vigorous shaking, with 25-ml portions of 10% alcohol until the wash water is neutral to phenolphthalein, and discard the washings. Transfer the ether extract to a tared beaker, and rinse the separator with 10 ml of ether, adding the rinsings to the beaker. Evaporate the ether on a steam bath just to dryness, and dry the residue to constant weight, preferably at 75° to 80° under a vacuum of not more than 200 mm of Hg , or at 100° at ambient pressure for 30 min. Cool in a desiccator, and weigh to obtain the uncorrected weight of unsaponifiable matter.

Determine the quantity of fatty acids in the residue as follows: Dissolve the residue in 50 ml of warm alcohol (containing phenolphthalein TS and previously neutralized with sodium hydroxide to a faint pink colour), and titrate with 0.02N sodium hydroxide to the same colour. Each ml of 0.02N sodium hydroxide is equivalent to 5.659 mg of fatty acids, calculated as oleic acid. Subtract the calculated weight of fatty acids from the weight of the residue to obtain the corrected weight of unsaponifiable matter in the sample.

Acid value

Weigh accurately about 1 g of the sample and dissolve in about 20 ml of hot 95% ethanol, previously neutralized in the presence of 0.5 ml of phenolphthalein TS. Cool the solution, then neutralize by titration with 0.01N ethanolic potassium hydroxide.

$$\text{Acid value} = \frac{0.561 \times \text{titration value (ml)}}{\text{sample weight (g)}}$$

Retain the neutralized solution for the Assay.

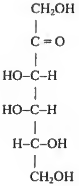
METHOD OF ASSAY

Add exactly 50 ml of 0.1N ethanolic potassium hydroxide solution to the neutralized solution obtained above from the determination of the acid value and bring to a steady boil for 2 min. Cool the solution and titrate the excess of potassium hydroxide with B ml of 0.1N hydrochloric acid. Perform a blank determination (= A ml of 0.1N hydrochloric acid).

$$\text{Ester value} = \frac{5.61 \times (A - B)}{\text{weight of sample (g)}}$$

D-TAGATOSE

New specifications prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000). No ADI was allocated at the 55th JECFA (2000).

SYNONYMS	D-*lyxo*-hexulose
DEFINITION	D-Tagatose is a ketohexose, an epimer of D-fructose inverted at C-4, with a sweet taste. It is obtained from D-galactose by isomerization under alkaline conditions in the presence of calcium.
Chemical names	D-Tagatose
C.A.S. number	87-81-0
Chemical formula	$C_6H_{12}O_6$
Structural formula	 $\begin{array}{c} CH_2OH \\ \vert \\ C=O \\ \vert \\ HO-C-H \\ \vert \\ HO-C-H \\ \vert \\ H-C-OH \\ \vert \\ CH_2OH \end{array}$
Formula weight	180.16
Assay	Not less than 98% on the dry basis
DESCRIPTION	Virtually odourless, white or almost white crystals
FUNCTIONAL USES	Sweetener, texturizer, stabilizer, humectant, formulation aid
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Very soluble in water, very slightly soluble in ethanol
Specific rotation (FNP 5)	$[\alpha]_D^{20}$: - 4 to - 5.6° (1% aqueous solution)
Melting range (FNP 5)	133 – 137°
Reaction with alkaline cupric tartrate	Proceed as directed for the measurement of reducing substances (Method II). A copious red precipitate of cuprous oxide is formed.
Chromatography	The retention time for the major peak in the chromatogram of the sample solution corresponds to that for D-tagatose in the chromatogram of reference standard D-tagatose (available from Arla Foods Ingredients amba, Skanderborgvej 277, 8260 Viby, Denmark) using the conditions described in the METHOD OF ASSAY.
PURITY	
Loss on drying (FNP 5)	Not more than 0.5% (102°, 2 h)
Total ash (FNP 5)	Not more than 0.1%

Lead (FNP 5)

Not more than 1mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental methods".

METHOD OF ASSAY

Determined by liquid chromatography (FNP5) using the following procedure.

Preparation of sample solution: Weigh accurately about 50 mg of dry sample into a 10-ml volumetric flask and add about 8 ml of purified, deionized water. Bring sample to complete dissolution and dilute to mark with purified deionized water. Filter through a 0.2 µm filter.

Preparation of reference solution: Use dry standard D-tagatose. Prepare a solution of the reference material as described for the sample solution.

Apparatus: Liquid chromatograph equipped with a refractive index detector and an integrator.

Conditions
Column: Biorad Aminex HPX-87C (length 30 cm, diameter 7.8 mm, particle size 9 µm) or equivalent
Column temperature: 85°
Mobile phase: Deionized water with 50 ppm calcium acetate
Flow rate: 0.6 ml/min
Injection volume: 20 µl

Procedure: Separately inject equal volumes of the sample solution and the reference solution into the chromatograph. Record the chromatograms and measure the response of D-tagatose peak. Calculate the content of D-tagatose in the sample solution by the following formula:

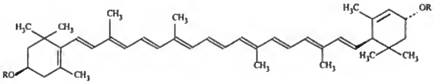
$$\%\ \text{D-Tagatose} = 100\,(A_S/A_R)\,(W_R/W_S)$$

Where
A_S = Peak area of sample solution
A_R = Peak area of reference solution
W_S = Weight of dry sample (mg)
W_R = Weight of dry reference standard (mg)

TAGETES EXTRACT
(Tentative)

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 31st JECFA (1987) and published in FNP 38 (1988) and in FNP 52 (1992). No ADI was allocated at the 31st JECFA (1987).

Information required on composition of commercial products, test for identification of xanthophylls and method of assay. Comments on other aspects of the monograph are invited.

SYNONYMS	Xanthophylls
DEFINITION	The major colouring principles are lutein and its dipalmitate (helenien), obtained by hexane extraction of dried petals of *Tagetes erecta* L with subsequent removal of the solvent. Other hydroxy derivatives of carotenes may be present together with other oxyderivatives such as epoxides; may contain fats, oils and waxes naturally occurring in the plant material together with edible vegetable oils added after the extraction.
Chemical names	Lutein: β,ε-Carotene-3,3'-diol, Helenien: Lutein dipalmitate; β,ε-Carotene-3,3'-diol dipalmitate
C.A.S. number	127-40-2 (lutein)
Chemical formula	Lutein: $C_{40}H_{56}O_2$ Helenien: $C_{72}H_{116}O_4$
Structural formula	 H3C CH3 CH3 CH3 H3C OR RO CH3 CH3 CH3 H3C CH3 Lutein: R = H Helenien: R = $CH_3(CH_2)_{14}CO$
Formula weight	Lutein: 568.88 Helenien: 1045.71
Assay	Content of total colouring matter (calculated as lutein) not less than declared
DESCRIPTION	Dark yellow-brown liquid
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water; soluble in hexane
Spectrometry	An acetone solution of the sample shows maximum absorption at about 444 nm
Xanthophylls	Information required
PURITY	
Residual solvent (FNP 5)	Hexane: not more than 50 mg /kg

Lead	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described on FNP 5, "Instrumental methods".
METHOD OF ASSAY	Information required

TALC

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding specifications prepared at the 51st JECFA (1998) and published in FNP 52 Add 6 (1998). An ADI "Not specified" was established at the 30th JECFA (1986).

SYNONYMS

Talcum; INS No. 553(iii)

DEFINITION

Naturally occuring hydrous magnesium silicate containing varying proportions of such associated materials as alpha-quartz, calcite, chlorite, dolomite, magnesite and phlogopite. Talc derived from deposits that are known to contain associated asbestos is not food grade.

C.A.S. number

14807-96-6

DESCRIPTION

Odourless, very fine, white or greyish white crystalline powder; unctuous, adheres readily to the skin, free from grittiness.

FUNCTIONAL USES

Anticaking agent, filter aid, coating agent, surface-finishing agent, texturizing agent, component of chewing gum base.

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)

Insoluble in water and ethanol

Infrared absorption

The infrared absorption spectrum of a potassium bromide dispersion of the sample exhibits major peaks as follows:

3677 ± 2 cm^{-1}	OH group
1018 ± 2 cm^{-1}	Si-O-Si group
669 ± 2 cm^{-1}	MgO-Si group

X-Ray diffraction

The X-ray diffraction pattern of a random powder sample exhibits reflections at d values of 9.34 Å, 4.66 Å and 3.12 Å

PURITY

Loss on ignition (FNP 5)

Not more than 9%
Accurately weigh 1 g sample into a tared platinum crucible, cover crucible, apply heat gradually and ignite for at least 3 h to a constant weight.

Loss on drying (FNP 5)

Not more than 0.5% (105 °, 1 h)

Water-soluble substances

Not more than 0.2%
Boil 20 g sample with 200 ml of water in a 250 ml beaker for 15 min., stir to avoid spurting. Cool to room temperature, transfer the contents to a 250 ml volumetric flask, rinse beaker with 25 ml water, add rinsings to the volumetric flask and make up to volume. Allow the mixture to stand for 15 min. and filter (use filtrate for the determination of water-soluble iron, below). Evaporate 100 ml of this solution, representing 8 g of talc, in a tared platinum dish on a steam bath to dryness and ignite gently to constant weight. The weight of the residue does not exceed 16 mg.

Water-soluble iron

Slightly acidify with hydrochloric acid TS the remaining half of the filtrate obtained in the test for water-soluble substances (above) and add 1 ml of potassium ferrocyanide TS. The solution does not turn blue.

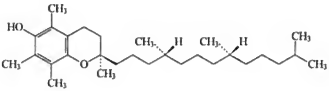
Acid-soluble substances

Not more than 2.5 %
Accurately weigh 2 g sample into a beaker, add 25 ml water and 10 ml of hydrochloric acid. Digest the sample on a hot plate for 15 min. taking care to avoid spurting of sample. Cool, transfer the contents into a 50 ml volumetric flask, rinse the beaker with water, add rinsings to the volumetric flask and make up to volume. Mix

	the contents and filter. To 20 ml of the filtrate in a tared platinum dish, add 2 ml of 2N sulfuric acid, evaporate to dryness and ignite to a constant weight. The residue does not exceed 20 mg.
Lead	Not more than 2mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of preparation may be used on the principles of the methods described in FNP 5, "Instrumental Methods".

d-α-TOCOPHEROL, CONCENTRATE

Prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000), superseding tentative specifications prepared at the 30th JECFA (1986) and published in FNP 37 (1986) and in FNP 52 (1992). A Group ADI of 0.15-2 mg/kg bw for dl-α-tocopherol and d-α-tocopherol, concentrate, singly or in combination, was established at the 30th JECFA (1986).

SYNONYMS	Vitamin E, *RRR*-α -tocopherol, 5,7,8-trimethyltocol, (+)-α-Tocopherol; INS No.307
DEFINITION	d-α-Tocopherol, concentrate is a form of Vitamin E obtained by the vacuum steam distillation of edible vegetable oil products, comprising a concentrated form of d-α-tocopherol. It may contain an edible vegetable oil added to adjust the required amount of total tocopherols, and the content of d-α-tocopherol may be adjusted by suitable physical and chemical means.
Chemical names	(2R,4'R,8'R)-2,5,7,8-tetramethyl-2-(4',8',12'-trimethyltridecyl)-chroman-6-ol
C.A.S. number	No. 59-02-9 (Vitamin E)
Chemical formula	$C_{29}H_{50}O_2$
Structural formula	
Formula weight	430.71
Assay	Not less than 40% of total tocopherols, of which not less than 95% consists of d-α-tocopherol
DESCRIPTION	Brownish red to light yellow, nearly odourless, clear viscous oil, which oxidizes and darkens slowly in air and on exposure to light
FUNCTIONAL USES	Antioxidant, nutrient
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water; soluble in ethanol; miscible with ether
Chromatography	The retention time of the major peak in the chromatogram of the sample solution is the same as that of the standard solution, both relative to the internal standard, as obtained in the Assay.
Colour reaction	Dissolve about 0.05 g of the sample in 10 ml of absolute ethanol. Add, with swirling, 2 ml of nitric acid and heat at about 75° for 15 min. A bright red to orange colour develops
PURITY	
Specific rotation	$[\alpha]^{25}_{D}$: Not less than +24° See description under TESTS
Acidity	Dissolve 1 g of the sample in 25 ml of a mixture of equal volumes of ethanol and ether that has been neutralized to phenolphthalein TS with 0.1 N sodium hydroxide, add 0.5 ml

of phenolphthalein TS, and titrate with 0.1 N sodium hydroxide until the solution remains faintly pink after shaking for 30 sec. Not more than 1.0 ml of 0.1 N sodium hydroxide is required.

Lead

Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparetion may be based on the principles of the method described in FNP 5, "Instrumental methods".

TESTS

PURITY TESTS

Specific rotation

Transfer an accurately weighed sample, equivalent to about 100 mg of total tocopherols, to a separator, and dissolve it in 50 ml of ether. To the separator add 20 ml of a 10% solution of potassium ferricyanide in 0.8% sodium hydroxide solution, and shake for 3 min. Wash the ether solution with four 50-ml portions of water, discard the washings, and dry over anhydrous sodium sulfate.

Evaporate the dried ether solution on a water bath under reduced pressure or in an atmosphere of nitrogen until about 7 or 8 ml remain, and then complete the evaporation, removing the last traces of ether without the application of heat. Immediately dissolve the residue in 5 ml of isooctane, and determine the optical rotation. Calculate the specific rotation, using as c the concentration expressed as the number of g of total tocopherols, determined in the Assay, in 100 ml of the solution.

METHOD OF ASSAY

Gas Liquid Chromatographic Method (FNP 5)

Reagents and solutions:
Internal Standard Solution: Transfer about 600 mg of hexadecyl hexadecanoate, accurately weighed, to a 200-ml volumetric flask, dissolve in a solution containing 2 parts of pyridine and 1 part of propionic anhydride, dilute to volume with the solution, and mix.

Standard solution: Transfer 12-, 25-, 37-, and 50-mg portions of USP Alpha Tocopherol Reference Standard, accurately weighed, to separate 50-ml Erlenmeyer flasks having 19/38 standard-taper ground-glass necks. Pipet 25.0 ml of the Internal Standard Solution into each flask, mix, and reflux for 10 min. under water-cooled condensers.

Sample solution: Transfer about 60 mg of the sample, accurately weighed, to another 50-ml Erlenmeyer flask, pipet 10.0 ml of the Internal Standard Solution into the flask, mix, and reflux for 10 min. under a water-cooled condenser.

Chromatographic System
Use a gas chromatograph equipped with a flame-ionization detector and a glass-lined sample-introduction system or on-column injection. Under typical conditions, the instrument contains a 2-m x 4-mm borosilicate glass column packed with 2% to 5% methylpolysiloxane on 80- to 100-mesh acid-base washed siliconized chromatographic diatomaceous earth. The column is maintained isothermally between 240° and 260°, the injection port at about 290°, and the detector block at about 300°. The flow rate of dry carrier gas is adjusted to obtain a hexadecyl-hexadecanoate peak approximately 18 to 20 min after sample introduction when a 2% stationary phase is used, or 30 to 32 min when a 5% stationary phase is used. (Note: Cure and condition the column as necessary).

System Suitability
Chromatograph a suitable number of injections of the sample solution, as directed under Calibration, to assure that the resolution factor R, between the major peaks occurring at retention times of approximately 0.50 (δ-tocopherol propionate) and 0.63 (β- and γ-tocopheryl propionates), relative of hexadecyl hexadecanoate at 1.00, is not less than 2.5.

Calibration

Chromatograph successive 2- to 5-µl portions of each standard solution until the relative response factor F, for each is constant (i.e. within a range of approximately 2%) for three consecutive injections. If graphic integration is used, adjust the instrument to obtain at least 70% maximum recorder response for the hexadecyl hexadecanoate peak. Measure the areas under the first (α-tocopheryl propionate) and second (hexadecyl hexadecanoate) major peaks, and record the values as A_s and A_1, respectively. Calculate the factor F, for each concentration of $(A_s/A_1) \times (C_1/C_s)$, in which C_1 and C_s are the exact concentrations, in mg per ml, of hexadecyl hexadecanoate and of USP Alpha Tocopherol Reference Standard in the Standard Preparation, respectively. Prepare a relative response factor curve by plotting area of α-tocopheryl propionate versus relative response factor.

Procedure

Inject a suitable portion (2 to 5 µl) of the Assay Preparation into the chromatograph, and record the chromatogram. Measure the areas under the four major peaks occurring at relative retention times of 0.50, 0.63, 0.76, and 1.00, and record the values as A_δ, $A_{\beta+\gamma}$, A_α and A_1, corresponding to δ-tocopherol propionate, β- and γ-tocopheryl propionates, α-tocopheryl propionate, and hexadecyl hexadecanoate, respectively. Calculate the weight, in mg, of each tocopherol form in the sample by the following formulas:

δ-tocopherol = $(10C_1/F) \times (A_\delta/A_1)$

β- and γ-tocopherols = $(10C_1/F) \times (A_{\beta+\gamma}/A_1)$

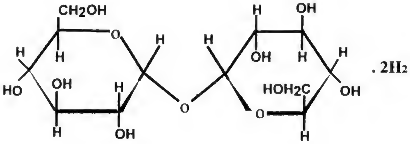
α-tocopherol = $(10C_1/F) \times (A_\alpha/A_1)$

where

F is obtained from the relative response factor curve (see Calibration) for each of the corresponding areas under the δ-, β- and γ-, and α-tocopheryl propionate peaks produced by the Assay Preparation. (NOTE: The relative response factors for δ-tocopheryl propionate and for β- and γ-tocopheryl propionates have been determined empirically to be the same as for α-tocopheryl propionate).

TREHALOSE

New specifications prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000). An ADI "not specified" was established at the 55th JECFA (2000).

SYNONYMS	α,α-trehalose
DEFINITION	A non-reducing disaccharide consisting of two glucose moieties joined together by an α-1,1 glucosidic bond. It is made from liquefied starch by a multistep enzymatic process. The commercial product is the dihydrate.
Chemical names	α-D-glucopyranosyl-α-D-glucopyranoside, dihydrate
C.A.S. number	6138-23-4
Chemical formula	$C_{12}H_{22}O_{11} \cdot 2H_2O$
Structural formula	
Formula weight	378.33
Assay	Not less than 98% on the dry basis
DESCRIPTION	White or almost white crystals
FUNCTIONAL USES	Texturizer, stabilizer, humectant, sweetener
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Soluble in water, slightly soluble in ethanol
Specific rotation (FNP 5)	$[\alpha_D^{20}$: +199° (5% aqueous solution)
Melting point	97°
PURITY	
Loss on drying (FNP 5)	Not more than1.5% (60°, 5h)
Total ash (FNP 5)	Not more than 0.05%
Lead	Not more than 1mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

METHOD OF ASSAY

Determine by liquid chromatography using the following conditions:

Sample preparation: Weigh accurately about 3g of dry sample into a 100ml volumetric flask and add about 80 ml of deionized water. Bring sample to complete dissolution and dilute to mark with deionized water. Filter through a 0.45 micron filter.

Preparation of standard solution: Dissolve accurately weighed quantities of dry standard reference trehalose (available from Hayashibara Co., Ltd, 2-3 Shimoishii 1-chome, Okayama 700, Japan) in water to obtain a solution having known concentration of about 30 mg of trehalose per ml.

Apparatus: Liquid chromatograph equipped with a refractive index detector and an integrating recorder.

Conditions:

Column and packing : Shodex Ionpack KS-801 or equivalent
-length : 300mm
-diameter : 10mm
-temperature : 50°C

Mobile phase : water

Flow rate : 0.4 ml/min

Injection volume : 8µl

Procedure: Separately inject equal volumes of the sample solution and the standard solution into the chromatograph. Record the chromatograms and measure the response of the trehalose peak. Calculate the quantity in mg of trehalose in 1 ml of the sample solution by the following formula:

$$\% \text{ trehalose} = 100 \times (R_U / R_S)\ (Ws/W_U)$$

where
R_S = Peak area of trehalose in the standard preparation
R_U = Peak area of trehalose in the sample preparation
W_S = Weight in mg of trehalose in the standard preparation
W_U = Weight of dry sample in mg

Section B. Specifications of certain flavouring agents

Organization of the section for specifications of flavouring agents

At its 44th meeting JECFA considered a new approach to the safety evaluation of flavouring agents. This approach incorporates a series of criteria whose use enables the evaluation of a large number of these agents in a consistent and timely manner. At the current session of the Committee specifications of identity and purity were prepared for 344 flavouring agents (220 revised specifications, page 128-159, 124 new specifications, page 160-177).

The specifications are presented in a tabular format because with the number of flavouring agents now being evaluated, the method of presentation becomes a matter of efficiency.

Information on specifications is given under the following headings, most of which are self-explanatory:

Name; Chemical name (Systematic name); Synonyms; Flavour and Extract Manufacturers' Association of the United States (FEMA) No; Council of Europe (COE) No; Chemical Abstract Service Registry (CAS) No; Molecular weight; Chemical formula; Physical form/odour; Solubility; Solubility in ethanol, Boiling point (information only); Identification test (ID), IR infrared spectrum; Assay min% (see page 199-201; Gas chromatographic (GC) assay of flavouring agents); Acid value max; Refractive index (at 20°, if not otherwise stated); Specific gravity (at 25°, if not otherwise stated); Other requirements, e.g. additional tests; the JECFA Session at which the specifications were prepared / the status of the specification. R means "specifications revised", S means "existing specifications maintained, S,T means "existing tentative specifications maintained", (further information), N means "new specifications", and N,T means "new tentative specifications, (further information required).

Chemical names of the new specifications are systematic names to be in harmony with the substance names used in the WHO Technical Report Series. When more than one systematic name exists, the systematic name which is listed is the closest to the name in the first column .

The last column indicates the data (information) required for the tentative specifications. Abbreviations for "data required" are as follows:

A=assay minimum, A(e)=equivalence factor for assay*, A(m)=details of assay method, BP=boiling point, ID=identity test, Low assay=quantitative information on by-products, RI=refractive index, SG=specific gravity. *A(e) is an equivalence factor to convert an assay obtained by aldehyde / ketone determination, ester determination, total alcohols determination, or titration determination to the % value which would be obtained if GC had been used for the assay (FNP 5).

The infrared and other spectra, used for identification and comparison purposes, are provided from page 179 onwards.

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
1	Allyl propionate	2-Propenyl propanoate	Allyl propionate	2040	2094	2408-70-0	114.15	$C_6H_{12}O_2$	Colourless liquid with a sharp sour apple/apricot odour
10	Allyl tiglate	2-Propenyl trans-2-methyl-2-butenoate	Allyl tiglate	2043	2183	7493-71-2	140.18	$C_8H_{12}O_2$	Colourless to pale yellow liquid with mild green fruity/green berry odour
17	Allyl phenylacetate	2-Propenyl phenylacetate	Allyl alpha-toluate	2039	2162	1797-74-6	176.22	$C_{11}H_{12}O_2$	Colourless, slightly viscous liquid with a honey-like odour
19	Allyl cinnamate	2-Propenyl 3-phenyl-2-propenoate	Allyl beta-phenylacrylate; Propenyl cinnamate; 2-Propen-1-yl 3-phenyl-2-propenoate; Vinyl carbinyl cinnamate	2022	334	1866-31-5	188.22	$C_{12}H_{12}O_2$	Colourless to light yellow, slightly viscous liquid with a peach/apricot odour
20	Allyl anthranilate	2-Propenyl 2-aminobenzoate		2020	254	7493-63-2	177.21	$C_{10}H_{11}NO_2$	Colourless to pale yellow liquid with a sharp heavy grape-like sweet odour and a green topnote
21	Allyl 2-furoate	2-Propenyl furan-2-carboxylate	Allyl pyromucate	2030	360	4208-49-5	152.15	$C_8H_8O_3$	Colourless or pale straw liquid which darkens when exposed to air and daylight: has a caramelic, fruity odour
36	Ethyl undecanoate	Ethyl undecanoate	Ethyl undecylate	3492	10633	627-90-7	214.35	$C_{13}H_{26}O_2$	Colourless liquid with a wine-like, fatty/fruity, somewhat nutty odour
39	Ethyl hexadecanoate	Ethyl hexadecanoate	Ethyl palmitate	2451	634	628-97-7	284.49	$C_{18}H_{36}O_2$	Colourless crystals with a waxy odour
40	Ethyl octadecanoate	Ethyl octadecanoate	Ethyl stearate	3490	745	111-61-5	312.54	$C_{20}H_{40}O_2$	Colourless, odourless mass
41	Ethanol	Ethanol	Ethyl alcohol	2419		64-17-5	46.07	C_2H_6O	Clear, colourless, mobile liquid with a characteristic odour and a burning taste
47	Isoamyl octanoate	3-Methylbutyl octanoate	Isoamyl caprylate	2080	401	2035-99-6	214.35	$C_{13}H_{26}O_2$	Colourless liquid with a fruity odour
48	Isoamyl nonanoate	3-Methylbutyl nonanoate	Isoamyl nonylate	2078	391	7779-70-6	228.37	$C_{14}H_{28}O_2$	Colourless oily liquid with a nutty, oily, apricot-like odour
51	Isoamyl 2-methylbutyrate	3-Methylbutyl 2-methylbutanoate	Isoamyl 2-methyl butanoate	3505	10721	27625-35-0	172.27	$C_{10}H_{20}O_2$	Colourless liquid with a fruity odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
1	-	-	122-123°	IR	99%	-	1.4105	0.914 at 20°		55th/R	
10	Slightly soluble in water, ether and most fixed oils	-	153	[req.]	98	1.0	1.451 - 1.454	0.939 - 0.943		55th/R,T	ID
17	-	-	89-93° at 3mm Hg	IR	99	-	1.5122 at 13.5°	1.033-1.041		55th/R	
19	insoluble in water; soluble in oils	Miscible	286	IR	97%	1.0	1.562-1.569	1.050-1.056		55th/R	
20	Almost insoluble in water, soluble in essential oils, poorly soluble in propylene glycol	-	105° at 2mm Hg	IR	98%	-	1.569-1.577	1.12		55th/R	
21	-	-	206-209°	IR	98	-	1.4945	1.181 (23°)	None	55th/R	
36	Soluble in ethanol and oils, insoluble in water	-	255°	IR	98%	-	1.438	0.87		55th/R	
39	Soluble in ethanol and oils, insoluble in water	-	303°	IR	99	1.0	1.404 - 1.408	0.863 - 0.865	Melting point 24-26°	55th/R	
40	Soluble in ethanol and oils, insoluble in water	-	105° at 11mm Hg	IR	89% (min. 96% ethyl esters of octadecanoate, palmitic and other fatty acids)	1.0	1.420 - 1.440	0.880 - 0.900	Melting point: 33-38°	55th/R	
41	Soluble in water	-	78°	IR	95	0.003	1.364	< 0.810	None	55th/R	
47	Slightly soluble in propylene glycol, insoluble in glycerol and water	1ml in 7ml 80% ethanol	267-268°	IR	98	1.0	1.425 - 1.429	0.855 - 0.861		55th/R	
48	Soluble in ethanol, insoluble in water	-	260°-265°	IR	96%	-	1.427-1.431	0.86		55th/R	
51	Soluble in ethanol and oil, insoluble in water	-	70-71°at 8mm Hg	[req.]	95	-	1.4124	0.852-0.861		55th/R,T	ID

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
58	Geranyl acetate	3,7-Dimethyl-2,6-octadien-1-yl acetate		2509	201	105-87-3	196.29	$C_{12}H_{20}O_{2}$	colourless liquid/floral odour
64	Rhodinyl propionate	3,7-Dimethyl-7-octen-1-yl propionate		2986	422	105-89-5	212.26	$C_{13}H_{24}O_{2}$	colourless, oily liquid/rose, geranium odour
69	Citronellyl valerate	3,7-Dimethyl-6-octen-1-yl pentanoate		2317	469	7540-53-6	240.39	$C_{15}H_{28}O_{2}$	liquid/rose, herb, honey-like odour
70	Geranyl hexanoate	trans-3,7-Dimethyl-2,6-octadien-1-yl hexanoate	Geranyl caproate	2515	317	10032-02-7	252.40	$C_{16}H_{28}O_{2}$	colourless liquid/rose-geranium, pineapple, banana odour
72	Geranyl isobutyrate	3,7-Dimethyl-2,6-octadienyl-2-methyl propanoate		2513	3061	2345-26-8	224.34	$C_{14}H_{245}O_{2}$	colourless to pale yellow liquid/rose odour
74	Rhodinyl isobutyrate	3,7-Dimethyl-7-octen-1-yl-2-methyl propanoate		2983	297	1338-23-8	226.36	$C_{14}H_{26}O_{2}$	colourlessto pale yellow oily liquid/fruity, floral odour
75	Geranyl isovalerate	3,7-Dimethyl-2,6-octadienyl-3-methylbutanoate		2518	448	109-20-6	238.37	$C_{15}H_{26}O_{2}$	colourless to pale yellow liquid/rose odour
77	Rhodinyl isovalerate	3,7-Dimethyl-7-octen-1-yl-3-methylbutanoate		2987	460	7778-96-3	240.26	$C_{15}H_{28}O_{2}$	colourless, oily liquid/rose odour
79	Formic acid	Formic acid		2487	1	64-18-6	46.03	$CH_{2}O_{2}$	colourless, highly corrosive liquid/characteristic pungent odour
80	Acetaldehyde	Acetaldehyde	Ethanal; Acetic aldehyde	2003	89	75-07-0	44.05	$C_{2}H_{4}O$	flammable, colourless liquiduid/pungent ethereal odour
81	Acetic acid	Acetic acid		2006	2	64-19-7	60.05	$C_{2}H_{4}O_{2}$	clear, colourless liquid/pungent odour
83	Propionaldehyde	Propanal		2923	90	123-38-6	58.08	$C_{3}H_{6}O$	colourless, mobile liquid/sharp, pungent odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
58	soluble in alcohol, most fixed oils; slightly soluble in propylene glycol; insoluble in glycerin, water	1 L in 9 ml 70% alcohol	240-245°	IR	90% (by ester determination)	-	1.458-1.464	0.900-0.914		55th/R,T	A(e)
64	soluble in alcohol; practically insoluble in water	-	255°	IR	95% (by ester determination)	-	1.457	0.910 (15.5°)		55th/R,T	A(e)
69	-	-	237°	IR	85% (min. 98% valerate esters of citronellol and related terpene alcohols)	-	1.4435	0.890 (15.5°)		55th/R	
70	-	-	240°	IR	95% (by ester determination)	-	1.45	0.890 (15.5°)		55th/R,T	A(e)
72	soluble in most organic solvents; insoluble in water	-	240°	IR	95% (by ester determination)	-	1.451-1.457	0.885-0.893 (d20/4)		55th/R,T	A(e)
74	soluble in alcohol; insoluble in water	-	260°	MS	95% (by ester determination)	-	1.448-1.453	0.881-0.891 (d20/4)		55th/R,T	A(e)
75	soluble in alcohol, most fixed oils; insoluble in water	-	279°	IR	95	-	1.454-1.470	0.878-0.899		55th/R	
77	soluble in alcohol; practically insoluble in water	-	270°	IR	95% (by ester determination)	-	1.447	0.8829 (15°)		55th/R,T	A(e)
79	miscible with water, alcohol, glycerin, ether	-	101°	IR	95%	-	1.366-1.376	1.2	Acetic acid: < 0.4%; Dilution Test: passes test; Heavy Metals: < 10 mg/kg; Sulfate: <0.004%	55th/R	
80	miscible with water, alcohol, organic solvents	-	21°	IR	99	5.0	1.360-1.380	0.804-0.811(0°/20°)	Res. on Evap.: 0.006%	55th/R	
81	miscible with water, alcohol, and glycerin	-	118°	IR	99.5	-	1.366-1.377	1.049	Heavy Metals: < 10 mg/kg; Nonvolatile Res.: < 0.005%; Readily Oxid. Sub.: Passes test; Solidification Pt.: > 15.6°	55th/R	
83	miscible with alcohol, ether, water	-	49°	IR	97	5.0	1.360-1.380	0.800-0.805	Dist. Range: 46° to 50°; Water: 2.5%	55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
84	Propionic acid	Propanoic acid		2924	3	79-09-4	74.08	C3 H6 O2	oily liquid/slightly pungent, rancid odour
85	Butyl alcohol	1-Butanol	Butan-1-ol	2178	52	71-36-3	74.12	C4 H10 O	colourless, mobile liquid/vinous odour
86	Butyraldehyde	Butanal	Butyl aldehyde	2219	91	123-72-8	72.11	C6 H8 O	colourless, mobile liquid/pungent, nutty odour
91	Hexyl alcohol	1-Hexanol	Alcohol C-6	2567	53	111-27-3	102.18	C6 H14 O	colourless, mobile liquid/mild, sweet, green
99	Octanoic acid	Octanoic acid	Caprylic acid	2799	10	124-07-2	144.21	C8 H16 O2	colourless, oily liquid/slight, unpleasant odour
105	Decanoic acid	Decanoic acid	Capric acid	2364	11	334-48-5	172.27	C10 H20 O2	white crystals/unpleasant, rancid odour
108	Undecanoic acid	Undecanoic acid	n-Undecylic acid	3245	696	112-37-8	186.29	C11 H22 O2	colourless crystals/ faint fatty, aldehydic odour
111	Lauric acid	Dodecanoic acid		2614	12	143-07-7	200.32	C12 H24 O2	white or faintly yellowish crystalline solid
113	Myristic acid	Tetradecanoic acid		2764	16	544-63-8	228.38	C14 H28 O2	hard, white, or faintly yellowish, somewhat glossy, crystalline solid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
84	miscible with water, alcohol, organic solvents	-	138.5-142.5°	IR	99.5	-	1.384-1.389	0.993-0.997 (20°/20°)	Dist. Range: 138.5° to 142.5°; Heavy Metals: <10 mg/kg; Nonvolatile Res.: <0.01%; Water: < 0.15%	55th/R	
85	miscible with alcohol, ether, organic solvents, 1 ml in 15 ml water	-	117.7°	IR	99.5	2.0	1.393-1.404	0.807-0.809	Butyl Ether: 0.15%; Dist. Range: max. 1.5° between beginning and end	55th/R	
86	soluble in 1 ml in 15 ml water; miscible with alcohol, ether	-	74.8°	IR	98	5.0	1.377-1.387	0.797-0.802	Dist. Range: 72° to 80°; para-Butyraldehyde. <2.5%; Water: <0.5%	55th/R	
91	miscible with alcohol, ether, 1 ml in 175 ml water	-	157	IR	96.5	2.0	1.415-1.420	0.816-0.821		55th/R	
99	slightly soluble in water; soluble in most organic solvents	-	240	IR	97%	366-396	1.423-1.429	0.91	Heavy Metals: < 10 mg/kg; Iodine Value: < 2.0; Res. on Ignition: < 0.1%. Saponification Value 366 to 398; Solidification Pt.: 8° to 15°; Unsaponifiable Matter: < 0.2%; Water: < 0.4%	55th/R	
105	soluble in most organic solvents; practically insoluble in water	-	268	IR	98%	320-329	n/a	n/a	Heavy Metals: < 10 mg/kg; Iodine Value: < 0.6; Res. on Ignition: < 0.1%; Saponification Value: 320-331; Solidification Pt.: 27° to 32°; Unsaponifiable Matter: < 0.2%; Water: < 0.2%	55th/R	
108	Insoluble in water; very soluble in alcohol, chloroform, acetone	-	284	IR	99	295-301	1.4355 (30°)	0.9948 (20°/20°)	Melting point: 33-38°	55th/R	
111	practically insoluble in water; soluble in alcohol, chloroform, ether	-	n/a	IR	98% by HPLC	252-287	n/a	n/a	Heavy Metals: < 10 mg/kg; Iodine Value: < 3.0; Res. on Ignition: <0.1%; Saponification Value: 253 to 287; Solidification Pt.: 26° to 44°; Unsaponifiable Matter: < 0.3%, Water: < 0.2%	55th/R,T	A(m)
113	practically insoluble in water; soluble in alcohol, chloroform, ether	-	n/a	IR	97% by titration	242-249	n/a	n/a	Heavy Metals: < 10 mg/kg; Iodine Value: < 1.0; Residue on Ignition: < 0.1%; Saponification Value: 242 to 251; Solidification Pt.: 48° to 55.5°; Unsaponifiable Matter: < 1%; Water: < 0.2%	55th/R,T	A(m)

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
115	Palmitic acid	Hexadecanoic acid		2832	14	57-10-3	256.43	C16 H32 O2	hard, white or faintly yellowish crystalline solid
116	Stearic acid	Octadecanoic acid		3035	15	57-11-4	284 48	C18 H36 O2	hard, white or faintly yellowish crystalline solid/tallow odour
121	Heptyl formate	Heptyl formate		2552	341	112-23-2	144 21	C8 H16 O2	colourless liquid with a fruity, floral, orris-rose odour
133	Lauryl acetate	Dodecyl acetate	Acetate C-12, Dodecyl acetate	2616	200	112-66-3	228.37	C14 H28 O2	colourless liquid with a waxy, citrus-rose odour
140	2-Ethylbutyl acetate	2-Ethylbutyl acetate		2425	215	10031-87-5	144 21	C8 H16 O2	liquid
147	cis-3 & trans-2-Hexenyl propionate	cis-3 & trans-2-Hexenyl propanoate		3778	10683	33467-74-2	156 23	C9 H16 O2	colourless to pale yellow liquid
154	Heptyl butyrate	Heptyl butanoate		2549	504	5870-93-9	186.30	C11 H22 O2	colourless liquid with a camomile odour
155	Octyl butyrate	Octyl n-butyrate		2807	272	110-39-4	200.32	C12 H24 O2	colourless liquid with a green herbaceous, parsley odour
156	Decyl butyrate	Decyl butyrate		2368	273	5454-09-1	228.37	C14 H28 O2	oily liquid with an ethereal, apricot odour
165	cis-3-Hexenyl hexanoate	cis-3-Hexen-1-ol hexanoate	cis-3-Hexenyl caproate	3403	11779	31501-11-8	198 31	C12 H22 O2	colourless to pale yellow liquid with a fruity green odour
166	Isobutyl hexanoate	2-Methylpropyl hexanoate	Isobutyl caproate	2202	314	105-79-3	172.27	C10 H20 O2	clear, colourless to yellowish liquid with a fruity, cocoa odour
168	Propyl heptanoate	Propyl heptanoate	Propyl heptoate	2948	367	7778-87-2	172.27	C10 H20 O2	colourless liquid with an ethereal odour
169	Butyl heptanoate	Butyl heptanoate	Butyl heptoate; butyl heptylate	2199	363	5454-28-4	186.30	C11 H22 O2	colourless liquid with a herbaceous, slightly fruity odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
115	practically insoluble in water; soluble in alcohol, ether, chloroform	-	n/a	IR	97% by HPLC	204-220	n/a	n/a	Heavy metals: <10 mg/kg; Iodine Value: < 2.0; Res. on Ignition: <0.1%; Saponification Value: 205 to 221; Solidification Pt.: 53.3o to 62o; Unsaponifiable Matter: <1.5%; Water: <0.2%	55th/R,T	A(m)
116	practically insoluble in water; soluble in alcohol, ether, chloroform	1 g in 20 ml alcohol	n/a	IR	98% by titration	196-211	n/a	n/a	Melting point: 64° (minimum); Heavy metals: < 10 mg/kg; Iodine Value: < 7; Res. on Ignition: < 0.1%; Saponification Value: 197 to 212; Solidification Pt.: 54.5° to 69°; Unsaponifiable Matter: < 1.5%; Water: < 0.2%	55th/R,T	A(m)
121	soluble in ether, most organic solvents; insoluble in water	1 ml in 5 ml 70% alcohol	176.7-178°	IR	94% (min. 99% heptyl formate + heptanal)	-	1.414	0.88277 (15°)		55th/R	
133	soluble in most organic solvents	1 ml in 4 ml 80% alcohol	150 (15 mmHg)	IR	98	1.0	1.410-1.436	0.860-0.865		55th/R	
140	-	-	160-163°	IR	98%	-	1.4109	0.8784 (20°)		55th/R	
147	-	-	169	IR	96	3.0	1.424-1.436	0.887-0.910		55th/R	
154	soluble in alcohol propylene glycol; insoluble in water	-	226°	IR	98%	-	1.4231	0.8555 (30°/30°)		55th/R	
155	soluble in alcohol; practically insoluble in water	-	244°	IR	97%	-	1.421-1.434	0.8549 (30°)		55th/R	
156	-	-	270°	IR	97%	-	1.4245-1.43977	0.8617 (20°)		55th/R	
165	soluble in alcohol, propylene glycol, most fixed oils, insoluble in water	-	122 (12 mmHg)	IR	96	-	1.420-1.440	0.870-0.890		55th/R	
166	-	1 ml in 2 ml 80% alcohol	200	IR	98	1.0	1.410-1.418	0.854-0.858		55th/R	
168	soluble in most organic solvents, insoluble in water	-	206-208°	IR	98%	-	1.4160-1.41894	0.85705 (20°)		55th/R	
169	soluble in most organic solvents	-	226.2°	IR	98%	-	1.4228	0.8555 (20°)		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
171	Octyl heptanoate	Heptanoic acid, octyl ester	Octyl heptoate	2810	366	5132-75-2	242.41	C15 H30 O2	colourless liquid with a fruity, slightly fatty odour
172	Isobutyl heptanoate	2-Methylpropyl heptanoate	Isobutyl heptoate	2200	364	7779-80-8	186.30	C11 H22 O2	colourless liquid with a green odour
176	Heptyl octanoate	Heptyl octanoate	Heptyl caprylate	2553	399	4265-97-8	242.41	C15 H30 O2	colourless, oily liquid with a green odour
177	Octyl octanoate	Octyl octanoate	Octyl caprylate	2811	395	2306-88-9	256.44	C16 H32 O2	colourless liquid with a faint, green tea odour
178	Nonyl octanoate	Nonyl octanoate	Nonyl caprylate	2790	396	7786-48-3	270.46	C17 H34 O2	colourless, oily liquid with a sweet, rose, mushroom odour
182	Isoamyl laurate	3-Methylbutyl dodecanoate	Isopentyl laurate	2077	379	6309-51-9	270.46	C17 H34 O2	Colourless, oily liquid with a faint oily, fatty odour
184	Butyl stearate	Butyl octadecanoate		2214	2189	123-95-5	340.59	C22 H44 O2	colourless, waxy solid, odourless or with a faintly fatty odour
193	Dodecyl isobutyrate	Dodecyl-2-methyl propanoate		3452	10563	6624-71-1	256.43	C16 H32 O2	liquid/slightly fruity or practically odourless
204	2-Methylbutyl 3-methylbutanoate	2-Methylbutyl-3-methylbutanoate		3506	10772	2445-77-4	162.26	C10 H20 O2	colourless liquid
206	Ethyl 2-methylbutyrate	Ethyl-2-methylbutanoate		2443	265	7452-79-1	130.19	C7 H14 O2	colourless liquid/strong, green-fruity, apple-like odour
207	n-Butyl 2-methylbuytyrate	Butyl-2-methylbutanoate		3393	10534	15706-73-7	158.23	C9 H18 O2	colourless to pale yellow liquid
208	Hexyl 2-methylbutanoate	Hexyl-2-methylbutanoate	Hexyl 2-methylbutyrate	3499	11781	10032-15-2	186.29	C11 H22 O2	colourless liquid/strong, fresh-green, fruity odour
209	Octyl 2-methylbutyrate	Octyl-2-methylbutanoate		3604	10866	29811-50-5	214.30	C13 H26 O2	colourless liquid
210	Isopropyl 2-methylbutyrate	1-Methylethyl-2-methylbutanoate		3699		66576-71-4	144.21	C8 H16 O2	colourless liquid
211	3-Hexenyl 2-methylbutanoate	3-Hexenylethyl-2-methylbutanoate		3497	2345	10094-41-4	184.28	C11 H20 O2	clear, colourless liquid
213	Methyl 2-methylpentanoate	Methyl-2-methyl pentanoate		3707		2177-77-7	130.19	C7 H14 O2	pale yellow liquid
214	Ethyl 2-methyl pentanoate	Ethyl-2-methyl pentanoate		3488	10616	28959-02-6	144.21	C8 H16 O2	colourless to pale yellow liquid
215	Ethyl 3-methylpentanoate	Ethyl-3-methyl pentanoate		3679		5870-68-8	144.21	C8 H16 O2	colourless liquid
216	Methyl 4-methylvalerate		Methyl isobutyl acetate	2721	322	2412-24-1	130.18	C7 H14 O2	colourless liquid/sweet, pineapple-like odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
171	soluble in most organic solvents, insoluble in water	-	290.8°	IR	98%	-	1.43488	0.85200 (20°)		55th/R	
172	soluble in most organic solvents	-	209°	IR	98%	-	[req.]	0.8593 (20°)		55th/R,T	RI
176	insoluble in water	1 ml in 3 ml 90% alcohol	291°	IR	98%	-	1.434	0.8520 (30°)	Melthing Pt.: -10°	55th/R	
177	soluble in alcohol; insoluble in water	-	306-307°	IR	98%	-	1.4352-1.4925	0.8554	Melting point -18°	55th/R	
178	soluble in alcohol, insoluble in water	-	315°	IR	99%	-	[req.]	0.86		55th/R,T	RI
182	soluble in alcohol; insoluble in water	-	190 (20 mmHg)	[req.]	97%	-	1.400-1.405	0.853-0.859		55th/R,T	ID
184	-	-	343°; (220-225° at 25 mmHg)	IR	99% (by ester determination)	-	n/a	0.855-0.875	Melting point 25°; Iodine Value: < 1; Saponification Value: 165° to 180°	55th/R,T	A(e)
193	soluble inorganic solvents; in soluble inwater	-	299	IR	97	1.0	1.432-1.436	0.854-0.860 (20°/20°)		55th/R	
204	-	-	113-115	IR	98%	-	1.394	0.852-0.857		55th/R	
206	soluble in alcohol, propylene glycol; very slightly soluble in water; miscible with most fixed oils	-	133	IR	95	2.0	1.393-1.400	0.863-0.870		55th/R	
207	-	-	180	IR	95%	-	1.402-1.500	0.856-0.866		55th/R	
208	soluble in alcohol, most fixed oils; insoluble in water	-	220	IR	95	2.0	1.416-1.421	0.854-0.859		55th/R	
209	-	-	250	IR	99.5	-	1.425	0.8577 (20°/20°)		55th/R	
210	insoluble in water	soluble	140	IR	98	-	1.395-1.399	0.847-0.855		55th/R	
211	-	-	212	IR	98	-	1.428-1.434	0.876-0.880		55th/R	
213	-	-	148	IR	98%	-	1.400-1.405	0.875-0.881		55th/R	
214	-	-	153	IR	96	1.0	1.401-1.404	0.859-0.865		55th/R	
215	-	-	159	IR	98%	-	1.405-1.412	0.866-0.873		55th/R	
216	soluble in alcohol, most fixed oils; insoluble in water	-	142-143	IR	97	-	1.402-1.406	0.885-0.892		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
218	Citric acid	2-Hydroxy-1,2,3-propane-tricarboxylic acid; 2-Hydroxy-1,2,3-propane-tricarboxylic acid, monohydrate				77-92-9	192.13	C6 H8 O7	White or colourless, odourless, crystalline solid. Monohydrate effloresces in dry air
222	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	2-Hydroxy-3-methyl-2-hexen-4-olide; 5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone		3153	2300	698-10-2	142.15	C7 H10 O3	yellow liquid with a maple, butterscotch odour
225	gamma-Heptalactone	4-Heptanolide; 5-Propyldihydro-2(3H)-furanone	Hepta-1,4-lactone	2539	2253	105-21-5	128.17	C7 H12 O2	colourless, slightly oily liquid with a coconut, sweet, malty, caramel odour
226	gamma-Octalactone	4-Octanolide; 5-Butyldihydro-2(3H)-furanone	Octa-1,4-lactone	2796	2274	104-50-7	142.20	C8 H14 O2	colourless to slightly yellow liquid with a sweet, coconut, fruity odour
227	4,4-Dibutyl-gamma-butyrolactone	4-Butyl-4-octanolide; 5,5-Dibutyldihydro-2(3H)-furanone	4-Butyl-4-hydroxyoctanoic acid lactone	2372	2231	7774-47-2	198.31	C12 H22 O2	colourless, oily liquid with a coconut-butter odour
228	delta-Octalactone	5-Octanolide; 6-Propyltetrahydro-2-pyrone	5-Hydroxyoctanoic acid lactone; Octa-1,5-lactone	3214	2195	698-76-0	142.20	C8 H14 O2	colourless to pale yellow liquid with a coconut-like odour
229	gamma-Nonalactone	4-Nonanolide; 5-Pentyldihydro-2(3H)-furanone	Nona-1,4-lactone; Aldehyde C-18, so-called	2781	178	104-61-0	156.22	C9 H16 O2	colourless to slightly yellow liquid with a coconut-like odour
232	delta-Decalactone	5-Decanolide; 6-Pentyltetrahydro-2-pyrona	Deca-1,5-lactone	2361	621	705-86-2	170.25	C10 H18 O2	colourless liquid with a coconut-fruity odour, butter-like on dilution
236	delta-Dodecalactone	5-Dodecanolide; 6-Heptyltetrahydro-2-pyrone	Dodeca-1,5-lactone	2401	624	713-95-1	198.31	C12 H22 O2	colourless to yellow liquid with a coconut-fruity odour, butter-like on dilution
239	omega-Pentadecalactone	15-Pentadecanolide; Oxacyclohexadecan-2-one	Pentadeca-1,5-lactone; Angelica lactone	2840	181	106-02-5	240.39	C15 H28 O2	white to pale yellow solid
240	omega-6-Hexadecenlactone	6-Hexadecenolide; Oxacycloheptadec-7-en-2-one	Ambrettolide; Hexadec-6-eno-1,16-lactone	2555	180	7779-50-2	252.39	C16 H28 O2	colourless to slightly yellow liquid with a strong, musk odour
241	epsilon-Decalactone	6-Decanolide; 7-Butyl-2-oxooxacycloheptane	Deca-1,6-lactone	3613		5579-78-2	170.25	C10 H18 O2	colourless to pale yellow liquid
242	epsilon-Dodecalactone	6-Dodecanolide; 7-Hexyl-2-oxooxacycloheptane	Dodeca-1,6-lactone	3610		16429-21-3	198.31	C12 H22 O2	colourless liquid with a sweet, fruity, peach odour
243	4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one	2-Hydroxy-3-methyl-2-penten-4-olide; 3-Hydroxy-4,5-dimethyl-2(5)-furanone	2,3-Dimethyl-4-hydroxy-2,5-dihydrofuran-5-one	3634	11834	28664-35-9	128.13	C6 H8 O3	clear, yellow liquid
244	3-Heptyldihydro-5-methyl-2(3H)-furanone	3-Heptyl-4-pentanolide; 3-Heptyldihydro-5-methyl-2(3H)-furanone		3350	10953	40923-64-6	198.31	C12 H22 O2	clear, colourless liquid
245	5-Hydroxy-2,4-decadienoic acid delta-lactone	2,4-Decadien-5-olide; 6-Pentyl-2-pyrone	Pentyl-alpha-pyrone	3696	10967	27593-23-3	166.22	C10 H14 O2	liquid with a mushroom, blue cheese lactone or dairy odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
218	Very soluble in water, slightly soluble in ether	Freely soluble	n/a	Positive test for citrate	99.5	-	n/a	n/a	Melting point: 152-154°; positive test for citrate	55th/R	
222	soluble in water	-	83-86 (0.5 mmHg)	IR	95	-	1.486-1.493	1.134-1.144		55th/R	
225	miscible with alcohol and most fixed oils	-	61-62 (2 mmHg)	IR	98	-	1.439-1.445	0.997-1.004(20°)		55th/R	
226	soluble in alcohol and slightly soluble in water	-	234	IR	95	8.0	1.443-1.447	0.970-0.980		55th/R	
227	insoluble in water; very slightly soluble in propylene glycol and soluble in alcohol	-	85 (0.5 mmHg)	IR	95%	-	1.451-1.455	0.937-0.943 (d204)		55th/R	
228	-	-	115-117 (12 mmHg)	IR	98	-	1.452-1.458	0.994-0.999		55th/R	
229	soluble in alcohol, most fixed oils and propylene glycol; insoluble in water	1 ml in 5 ml 60% alcohol	121-122 (6 mmHg)	IR	98	2.0	1.446-1.450	0.958-0.966		55th/R	
232	very soluble in alcohol and propylene glycol; insoluble in water	-	281	IR	98	5.0	1.456-1.459	0.964-0.971	Saponfication Value: 323 to 333	55th/R	
236	very soluble in alcohol, propylene glycol and vegetable oil; insoluble in water	-	140-141 (1 mmHg)	IR	98	8.0	1.458-1.461	0.942-0.950	Saponfication Value: 278 to 286	55th/R	
239	-	-	n/a	IR	98	1.0	n/a	n/a	Melting point 32°	55th/R	
240	-	1 ml in 9 ml 80% alcohol	185-190 (16 mm Hg)	IR	98	-	1.477-1.482	0.949-0.957		55th/S,T	SG range
241	-	-	117 (3 mmHg)	IR	99	-	1.458-1.463	0.976		55th/R	
242	slightly soluble in water, miscible with fats	-	150 (2 mmHg)	IR	99	-	1.459-1.463	0.950-0.958		55th/R	
243	-	-	81 (6 mm Hg)	IR	97.5	-	n/a	n/a	Melting point c 25°	55th/R	
244	-	-	170 (17 mmHg)	IR	[req.]	-	1.443-1.450	[req.]		55th/R,T	A, SG
245	soluble in fats, insoluble in water	-	85 (2.5 mm Hg)	IR	98.7	-	1.501-1.509	1.000-1.009		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
247	5-Hydroxy-7-decenoic acid delta-lactone	7-Decen-5-olide; 6-Pentyltetrahydro-2-pyrone	7-Decene-1,5-lactone; Jasmine lactone	3745		25524-95-2	168.24	$C_{10}H_{16}O_{2}$	colourless to light yellow liquid with a coconut, fatty, fruity, peach, jasmine, woody, balsamic odour
248	5-Hydroxy-8-undecenoic acid delta-lactone	8-Undecen-5-olide; 6-Hexyltetrahydro-2-pyrone		3758		68959-28-4	182.26	$C_{11}H_{18}O_{2}$	colourless liquid with a milky buttery odour
251	Isobutyl alcohol	2-Methylpropanol	Isobutanol	2179	49	78-83-1	74.12	$C_{4}H_{10}O$	colourless, mobile liquid with a penetrating, winey odour
252	Isobutyraldehyde	2-Methylpropanal		2220	92	78-84-2	72.11	$C_{4}H_{8}O$	colourless, mobile liquid with a sharp, pungent odour
256	2-Ethylbutyraldehyde	2-Ethylbutanal		2426	95	97-96-1	100.16	$C_{6}H_{12}O$	colourless, mobile liquid with a pungent odour
260	2-Methylpentanal	2-Methylpentanal	2-Methylvaleraldehyde	3413	706	123-15-9	100.15	$C_{6}H_{12}O$	colourless to pale yellow liquid
271	4-Methyloctanoic acid	4-Methyloctanoic acid	Isononanoic acid	3575	11926	54947-74-9	158.24	$C_{9}H_{18}O_{2}$	clear, colourless liquid with a goat, costus, mutton odour
298	2-Tridecanone	Tridecan-2-one	Methyl undecyl ketone	3388	11194	593-08-8	198.35	$C_{13}H_{26}O$	white to waxy mass or crystalline leaves with a milky, herbaceous, slightly spicy odour
299	2-Pentadecanone	Pentadecan-2-one	Methyl tridecyl ketone	3724	11808	2345-28-0	226.40	$C_{15}H_{30}O$	white to waxy mass or crystalline leaves
300	3-Methyl-2-butanol	3-Methylbutan-2-ol	Isopropyl methyl carbinol	3703		598-75-4	88.15	$C_{5}H_{12}O$	-
306	Isopropyl propionate	Isopropyl propionate		2959	404	637-78-5	116.16	$C_{6}H_{12}O_{2}$	liquid
308	Isopropyl hexanoate	Isopropyl hexanoate	Isopropyl caproate	2950	312	2311-46-8	158.24	$C_{9}H_{18}O_{2}$	colourless liquid
310	Isopropyl isovalerate	Isopropyl 3-methylbutanoate	Isopropyl isopentanoate	2961	445	32665-23-9	144.21	$C_{8}H_{16}O_{2}$	colourless to pale yellow liquid
311	Isopropyl myristate	Isopropyl tetradecanoate	Tetradecanoic acid; Isopropyl tetradecanoate	3556	386	110-27-0	270.46	$C_{17}H_{34}O_{2}$	colourless to pale yellow, odourless liquid
316	cis-3-Hexenal	(Z)-Hex-3-enal		2561	2008	6789-80-6	98.14	$C_{6}H_{10}O$	colourless liquid
317	3-Hexenoic acid	Hex-3-enoic acid	Hydrosorbic acid	3170	2256	4219-24-3	114.14	$C_{6}H_{10}O_{2}$	-

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
247	soluble in alcohol and ether; insoluble in water and fat	-	130 (3 mm Hg)	IR	95%	-	1.477	0.979-0.989		55th/R	
248	insoluble in water; soluble in fat	-	140	IR	95	-	1.473-1.480	0.97-0.99		55th/R	
251	miscible with alcohol, ether; soluble in water 1 ml in 140 ml	-	108	IR	98	2.0	1.392-1.398	0.799-0.801		55th/R	
252	miscible with alcohol, ether; soluble in water 1 ml in 125 ml	-	64	IR	98	5.0	1.369-1.379	0.783-0.788		55th/R	
256	miscible with alcohol, ether; soluble in water 1 ml in 50 ml	-	117	IR	95	2.0	1.400-1.405	0.808-0.814	Dist. Range: >95% between 100° and 120°	55th/R	
260	-	-	116	IR	97% (by aldehyde determination)	-	1.412	0.805-0.811		55th/R,T	A(e)
271	-	-	149 (22 mmHg)	IR	97%	-	1.433-1.440	0.900-0.908 (20°/20°)		55th/R	
298	soluble in alcohol, propylene glycol and oils; insoluble in water	-	162° (15 mmHg)	IR	95	10.0	1.432-1.438	0.817-0.823	Melting Point: 28-31°	55th/R	
299	soluble in alcohol, propylene glycol and oils; insoluble in water	-	134° (10 mm Hg)	IR	96	5.0	n/a	n/a	Melting point: 41°	55th/R	
300	-	-	112	IR	98%	-	1.406-1.412	0.815-0.821		55th/R	
306	completely miscible with alcohol and diluted alcohol	-	108-111	[req.]	98%	-	1.384-1.390	0.863-0.869 (20°)		55th/R,T	ID
308	almost insoluble in water; soluble in alcohol	-	176	MS	99	-	[req.]	0.854-0.860 (20°)		55th/R,T	RI
310	insoluble in water; soluble in most organic solvents	-	68-70° (55 mm Hg)	IR	95	-	1.394 - 1.399	1.376-1.379		55th/R	
311	insoluble in water and glycerol; soluble in alcohol	-	192 (22 mmHg)	IR	99%	2.0	1.432 - 1.437	0.847 - 0.855	Saponification Value: 205-211; Iodine Value: <=1	55th/R	
316	-	-	20° (20 mm Hg)	IR	97%	-	1.427-1.436	0.967-0.973		55th/R	
317	-	-	208	IR	95%	-	1.493-1.496	0.958-0.971		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
319	cis-4-Hexenal	(Z)-Hex-4-enal		3496	10337	4634-89-3	98.14	$C_{6}H_{10}O$	colourless liquid
320	cis-4-Heptenal	(Z)-Hept-4-en-1-al		3289	2124	6728-31-0	112.17	$C_{7}H_{12}O$	slightly yellow liquid with a fatty, green odour
324	cis-6-Nonen-1-ol	(Z)-Non-6-en-1-ol		3465	10294	35854-86-5	142.24	$C_{9}H_{18}O$	white to slightly yellow liquid with a powerful, melon-like odour
327	5&6-Decenoic acid (mixture)			3742		72881-27-7	170.25	$C_{10}H_{18}O_{2}$	colourless liquid with a bitter odour
329	9-Undecenal	Undec-9-en-1-al	Aldehyde C-11, Undecylenic aldehyde	3094	123	143-14-6	168.28	$C_{11}H_{20}O$	colourless, pale yellow, oily liquid
333	Oleic Acid	(Z)-Octadeca-9-enoic acid		2815	13	112-80-1	282.47	$C_{18}H_{34}O_{2}$	colourless to pale yellow, oily liquid with a characteristic lard-like odour
334	Methyl 3-hexenoate	Methyl hex-3-enoate		3364	10801	2396-78-3	128.17	$C_{7}H_{12}O_{2}$	colourless liquid
337	Methyl cis-4-octenoate	(Z)-Methyl oct-4-enoate		3367	10834	21063-71-8	156.22	$C_{9}H_{16}O_{2}$	-
338	Ethyl cis-4-octenoate	(Z)-Ethyl oct-4-enoate		3344	10619	34495-71-1	170.24	$C_{10}H_{18}O_{2}$	-
339	Ethyl cis-4,7-octadienoate	Ethyl (Z)-octa-4,7-dienoate		3682		69925-33-3	168.24	$C_{10}H_{16}O_{2}$	colourless liquid
340	Methyl 3-nonenoate	Methyl non-3-enoate		3710		13481-87-3	170.25	$C_{10}H_{18}O_{2}$	clear, colourless liquid
341	Ethyl trans-4-decenoate	Ethyl (E)-4-Decenoate		3642	10578	76649-16-6	198.31	$C_{12}H_{22}O_{2}$	-
342	Methyl 9-undecenoate	Methyl undec-9-enoate	Methyl undecylenate	2750	2101	5760-50-9	198.31	$C_{12}H_{22}O_{2}$	colourless to pale straw-yellow, oily liquid
344	Butyl 10-undecenoate	Butyl undec-10-enoate	Butyl undecylenate	2216	2103	109-42-2	240.39	$C_{15}H_{28}O_{2}$	colourless to pale yellow liquid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
319	slightly soluble in water; soluble in ethanol, phthalates, ethers and most fixed oils	-	73.5-75° (100 mm Hg)	MS	95	-	1.428-1.432	0.958-0.971		55th/R	
320	soluble in alcohol and most fixed oils; insoluble in water	-	60 (25 mmHg)	IR	98.0% as sum of (Z) and (E) isomers, <=93.0% (Z)	-	1.432-1.436	0.843-0.855		55th/R	
324	insoluble in water, soluble in fixed oils	-	85 (5 mmHg)	IR	95.0% (one major isomer)	-	1.448-1.450	0.844-0.851		55th/R	
327	insoluble in water, soluble in alcohol and fixed oils	-	58	IR	95 of 6:1 trans:cis isomer ratio	-	1.447-1.460	0.916-0.945		55th/R	
329	insoluble in water; soluble in alcohol	-	206	IR	[req.] / 30% (sum of cis and trans isomers)	-	1.442-1.446	0.841-0.850 (20°)		55th/R,T	A
333	insoluble in water, miscible in alcohol, ether, fixed oils	-	194-195 (1.2 mm Hg)	IR	90% (min. 99% oleic, palmitic and other fatty acids)	-	1.46	0.892-0.898	Melting point 13.4; Heavy Metals: <=10 mg/kg; Iodine Value: 83-103; Residue on Ignition: <=0.01%; Saponification Value: 196-206; Unsaponifiable Matter: <=2.0%; Water: <=0.4%	55th/R	
334	-	-	[req.]	IR	97	-	1.422-1.428	0.912-0.922 (20°)		55th/R,T	BP
337	soluble in ether	-	72° (11 mm Hg)	MS	[req.]	-	[req.]	[req.]		55th/R,T	A, RI, SG
338	-	-	79° (10 mm Hg)	MS	98	-	[req.]	[req.]		55th/R,T	RI, SG
339	-	-	88 (20 mmHg)	IR	95%	-	1.440-1.444	0.901-0.909 (20°)		55th/R	
340	insoluble in water	-	90 (15 mmHg)	IR	95%	-	1.432-1.442	0.860-0.900 (20°)		55th/R	
341	-	-	90° (3 mmHg)	IR	95%	-	1.432-1.444	0.877-0.883		55th/R	
342	insoluble in water; soluble in alcohol	-	247-248	IR	97%	-	1.435-1.441	0.886 (20°)	Melting point: 27.5°	55th/R	
344	-	-	125-128	[req.]	98%	-	1.439-1.445	0.872-0.878 (20°)		55th/R,T	ID

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
347	2-Methyl-3-pentenoic acid	2-Methyl pent-3-enoate		3464	10147	37674-63-8	114.15	C6 H10 O2	clear, colourless liquid
353	Ethyl 2-methyl-3,4-pentadienoate	Ethyl 2-methylpenta-3,4-dienoate		3678		60523-21-9	140.18	C8 H12 O2	-
354	Methyl 3,7-dimethyl-6-octenoate	Methyl 3.7-dimethyloct-6-enoate	Methyl citronellate	3361	10781	2270-60-2	184.28	C11 H20 O2	colourless liquid
363	Linalyl isovalerate	1,5-Dimethyl-1-ethenylhex-4-enyl 3-methylbutyrate	3,7-Dimethylocta-1,6-dien-3-yl isovalerate; Linalyl isopentanoate; Linalyl isovalerate, Linalyl 3-methylbutyrate	2646	449	1118-27-0	238.37	C15 H26 O2	colourless to pale yellow liquid with a sweet, fruity citrusy odour
365	Linalyl octanoate	1,5-Dimethyl-1-ethenylhex-4-enyl octanoate	3,7-Dimethyl-1,6-octadien-3-yl octanoate; Linalyl caprylate; Linalyl octoate; Linalyl octylate	2644	397	10024-64-3	280.46	C18 H32 O2	colourless, oily liquid
367	Terpinyl formate	p-Menth-1-en-8-yl formate		3052	348	2153-26-6	182.26	C11 H18 O2	colourless liquid with a floral citrusy, tart, herbaceous odour
370	Terpinyl butyrate	p-Menth-1-en-8-yl butyrate		3049	278	2153-28-8	224.34	C14 H24 O2	clear, colourless liquid
371	Terpinyl isobutyrate	p-Menth-1-en-8-yl isobutyrate	Terpinyl 2-methylpropionate	3050	300	7774-65-4	224.34	C14 H24 O2	clear, colourless liquid
372	Terpinyl isovalerate	p-Menth-1-en-8-yl isovalerate	Terpinyl isopentanoate; Terpinyl isovalerate; p-Menth-1-en-8-yl isopentanoate; p-Menth-1-en-8-yl 3-methylbutyrate	3054	456	1142-85-4	238.38	C15 H26 O2	colourless oily liquid with a peculiar sweet-piney, floral-incense-like citrus odour
373	p-Menth-3-en-1-ol	p-Menth-3-en-1-ol	Terpinen-1-ol	3563	10252	586-82-3	154.25	C10 H18 O	colourless, oily liquid with a dry-woody, piney and slightly musty odour
376	p-Menthan-2-ol		Carvomenthol	3562	2228	499-69-4	156.26	C10 H20 O	-
377	Dihydrocarvone	p-Menth-8-en-2-one		3565	11703	7764-50-3	152.24	C10 H16 O	almost colourless liquid with a herbaceous, spearmint-like odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
347	slightly soluble in water, soluble in alcohol and most fixed oils	-	85° (10 mm Hg)	[req.]	99 (as 60/40 mix of cis/trans isomers)	-	1.433-1.440	0.960-0.966		55th/R,T	ID
353	-	-	160	IR	98	-	1.446-1.452	0.922-0.928		55th/R	
354	-	-	88 (20 mmHg)	IR, MS	95%	-	1.437-1.443	0.897-0.907		55th/R	
363	insoluble in water, soluble in alcohol and oils	1 ml in 5.5 to 7 ml 80% alcohol	188	IR	96	0.09	1.448-1.453	0.880-0.888		55th/R	
365	insoluble in water; soluble in alcohol	-	264	IR	93% (min 98% octanoate esters of linalool and related terpene alcohols)	-	1.454-1.460	0.877-0.883		55th/R	
367	very slightly soluble in water	1 ml in 6 ml 60% alcohol	213-225	IR	95% (by ester determination)	-	1.467-1.473	0.987-0.993 (15.5°)		55th/R,T	A(e)
370	insoluble in water; soluble in alcohols and oils	-	244-246	[req.]	95% (by ester determination)	-	1.463-1.468	0.962-0.968 (15.5°)		55th/R,T	ID, A(e)
371	insoluble in water; soluble in alcohols and oils	-	242	IR	98	0.2	1.457-1.463	0.931-0.942		55th/R	
372	insoluble in water, soluble in alcohols	-	248	[req.]	95% (by ester determination)	-	[req.]	0.931-0.937		55th/R,T	ID, A(e), RI
373	Slighly soluble in water; soluble in alcohols and oils	-	210	MS	95%	-	1.478 (24°)	0.93		55th/R	
376	-	-	222	MS	95%	-	1.462-1.463	0.887-0.893		55th/R	
377	soluble in alcohol and most fixed oils; insoluble in water	-	220-222	IR	77% (min 97% dihydrocarvone + carvone + the corresponding alcohols)	-	1.470-1.474	0.923-0.928		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
380.2	l-Carvone	p-Mentha-6,8-dien-2-one	laevo-Carvone	2249	146	6485-40-1	150 22	$C_{10}H_{14}O$	(l-form) colourless to pale strawberry coloured liquid with a spearmint-like odour
383	Carvyl propionate	1-p-Mentha-6,8-dien-2-yl propionate		2251	424	97-45-0	208.30	$C_{13}H_{20}O_2$	colourless slightly oily liquid with a minty-spearminty herbaceous odour
392	beta-Ionol	4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-butene-2-ol		3625		22029-76-1	194.32	$C_{13}H_{22}O$	clear, colourless liquid
394	Dihydro-beta-ionone	4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-butan-2-one		3626		17283-81-7	194.32	$C_{13}H_{22}O$	colourless to pale yellow liquid
398	Methyl-alpha-ionone	5-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-4-penten-3-one	alpha-Cyclocitrylidene butanone; alpha-Cyclocitrylidene methyl ethyl ketone; alpha-n-Methylionone; Raldeine; alpha-Cetone	2711	143	127-42-4	206.33	$C_{14}H_{22}O$	yellowish, oily liquid
400	Methyl-delta-ionone	4-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-3-methyl-3-buten-2-one	beta-Isomethylionone, "delta"-Methylionone;Isomethyl-beta-ione	2713		7784-98-7	206.33	$C_{14}H_{22}O$	colourless to yellow liquid
402	1,4-Dimethyl-4-acetyl-1-cyclohexene	1,4-Dimethyl-4-acetyl-1-cyclohexene	1,4-Dimethylcyclohex-3-enyl methyl ketone	3449	11062	43219-68-7	152.24	$C_{10}H_{16}O$	colourless liquid
406	2-Acetoxy-3-butanone	1-Methyl-2-oxopropyl acetate	Butan-3-one-2-yl acetate; Acetoin acetate	3526	608	4906-24-5	130.14	$C_6H_{10}O_3$	colourless to slightly yellow liquid
407	Butan-3-one-2-yl butanoate	1-Methyl-2-oxopropyl butyrate	Acetoyl butyrate	3332	10525	84642-61-5	158.20	$C_8H_{14}O_3$	white to slightly yellow liquid with a sweet, red berry characteristic odour
409	3-Hydroxy-2-pentanone	3-Hydroxypentan-2-one	Acetyl ethyl carbinol	3550	11115	3142-66-3	102 13	$C_5H_{10}O_2$	-
411	4-Methyl-2,3-pentanedione	4-Methylpentane-2,3-dione	Acetyl isobutyryl	2730	2043	7493-58-5	114.14	$C_6H_{10}O_2$	yellow oil
412	2,3-Hexanedione	Hexane-2,3-dione	Acetyl-n-butyryl; Methyl propyl diketone	2558	152	3848-24-6	114.14	$C_6H_{10}O_2$	yellow, oily liquid with a butter-sweet odour
414	5-Methyl-2,3-hexanedione	5-Methylhexane-2,3-dione	2-Methyl-4,5-hexanedione; Acetyl isovaleryl; Isobutyl methyl diketone; Isobutyl methyl glyoxal, Acetyl isopentanoyl	3190	11148	13706-86-0	128.17	$C_7H_{12}O_2$	yellowish liquid oil with a butter odour
416	5-Hydroxy-4-octanone	5-Hydroxyoctan-4-one	5-Octanol-4-one; Butyroin	2587	2045	496-77-5	144.21	$C_8H_{16}O_2$	yellowish liquid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
380.2	soluble in propylene glycol and most fixed oils; insoluble in glycerol; miscible with alcohol	1 ml in 2 ml 70% alcohol	231	IR	97	-	1.495-1.499	0.956-0.960	Optical rotation: -62° to -57°	55th/R	
383	insoluble in water; soluble in alcohol and most fixed oils	-	239	IR	98%	-	1.469-1.479	0.942-0.962		55th/R	
392	-	-	107° (3 mm Hg)	IR	92% (min. 99% ionol and ionone isomers)	-	1.499	0.927-0.933		55th/R	
394	-	-	90° (0.2 mm Hg)	IR	99	-	1.479-1.485	0.920-0.930		55th/R	
398	-	-	238	IR	90% (minimum 95% sum of methyl ionone isomers)	-	1.498-1.503	0.921-0.930		55th/R	
400	insoluble in water; soluble in alcohol	-	232	IR	95.0% (sum of 4 isomers)	-	1.493-1.499	0.931-0.938		55th/R	
402	-	-	208-211	IR	98	-	1.468-1.473	0.930-0.936		55th/R	
406	soluble in ethanol	-	74-75° (20 mm Hg)	IR	98%	-	1.410-1.416	0.990-1.010		55th/R	
407	soluble in alcohol, propylene glycol and most fixed oils; insoluble in water	-	76° (11 mm Hg)	IR	96%	-	1.408-1.429	0.972-0.992		55th/R	
409	-	-	105-107° (50 mm Hg)	MS	[req.]	-	[req.]	[req.]		55th/R,T	A, RI, SG
411	-	-	116	MS	96%	-	1.397-1.405	0.941-0.950 (20°)	Melting point: - 2.4°	55th/R	
412	slightly soluble in water; soluble in propylene glycol, alcohol, and oils	-	128	IR	93% (min. 98% named cpd + methylpentanediones)	-	1.409-1.419	0.930-0.950		55th/R	
414	slightly soluble in water; miscible with alcohol, propylene glycol, and glycerol	-	138	IR	95%	-	1.408-1.414	0.908 (22°)		55th/R	
416	almost insoluble in water; soluble in alcohol	-	162	[req.]	95%	-	1.426-1.432	0.907-0.923 (20°)		55th/R,T	ID

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
417	2,3-Undecadione	Undeca-2,3-dione	Acetyl nonanoyl, Acetyl nonyryl, Acetyl pelargonyl	3090	155	7493-59-6	184.28	C11 H20 O2	oily, yellow liquid
418	Methylcyclo- pentenolone	3-Methylcyclopentane-1,2-dione	2-Hydroxy-3-methyl-2-cyclopenten-1-one; Cyclotene; Maple lactone	2700	758	80-71-7	112.13	C6 H8 O2	white, crystalline powder with a nutty odour, maple-liquorice aroma in dilute solution
420	3,4-Dimethyl-1,2-cyclopentanedione	3,4-Dimethylcyclopentane-1,2-dione		3268	2234	13494-06-9	126.16	C7 H10 O2	pale yellow to yellow powder
421	3,5-Dimethyl-1,2-cyclopentanedione	3,5-Dimethylcyclopentane-1,2-dione		3269	2235	13494-07-0	126.16	C7 H10 O2	light yellow to yellowish brown powder with a maple, burnt sugar odour
426	2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1-one	2-Hydroxy-3,5,5-trimethylcyclohex-2-en-1-one		3459	11198	4883-60-7	154.21	C9 H14 O2	colourless to pale yellow solid
433	l-Menthyl lactate			3748		59259-38-0	228.33	C13 H24 O3	colourless liquid or white crystalline solid with a weak chamomile or tobacco odour
438	5-Hydroxy-2-dodecenoic acid delta-lactone	2-Dodecen-5-olide; 6-Heptyl-2H-dihydro-2-pyrone		3802		16400-72-9	196.30	C12 H20 O2	clear, light yellow liquid
439	4-Carvomenthenol	p-Menth-1-en-4-ol	1-Methyl-4-isopropyl-1-cyclohexene-4-ol; Origanol; Terpineol; 4-Terpinenol	2248	2229	562-74-3	154.25	C10 H18 O	colourless, oily liquid with a warm-peppery, mildly earthy, musty-woody odour
441	4-Thujanol	2-Methyl-5-(1-methylethyl)bicyclo[3.1.0]hexan-2-ol	Sabinene hydrate	3239	10309	546-79-2	154.25	C10 H18 O	- / terpineol odour
446	dl-Menthone 1,2-glycerol ketal	1,4-Dioxaspiro[4,5]decane-2-menthanol	Frescolat, Type MGA Racemic	3808		63187-91-7	228.33	C13 H24 O3	clear colourless viscous liquid
451	Furfuryl alcohol	2-Hydroxymethylfuran		2491	2023	98-00-0	98.01	C5 H6 O2	colourless to yellow oily liquid with a faint burnt odour
456	1,4-Dithiane	1,4-Dithiane	p-Dithiane; 1,4-Dithiacyclohexane, Tetrahydro-1,4-dithiin; Diethylene disulfide	3831		505-29-3	120.24	C4 H8 S2	white to off-white crystals
458	Allyl sulfide	Diallyl sulfide	Thioallyl ether; 2-Propenyl sulfide, 3,3'-Thiobispropene	2042	11846	592-88-1	114.21	C6 H10 S	colourless to pale yellow liquid with garlic odour
462	4-(Methylthio)butanol	4-(Methylthio)-1-butanol		3600		20582-85-8	120.21	C5 H12 OS	sulfury,potato, or green vegetable odour
464	2-Methyl-4-propyl-1,3-oxathiane	2-Methyl-4-propyl-1,3-oxathiane		3578	11540	67715-80-4	160.28	C8 H16 OS	-

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
417	very slightly soluble in water; soluble in alcohol	-	109-111° (10 mm Hg)	MS	[req.]	-	[req.]	[req.]		55th/R,T	A, RI, SG
418	soluble in alcohol and propylene glycol; slightly soluble in most fixed oils and 1 g in 72 ml water	1 g in 5 ml 90% alcohol	n/a	IR	95%	-	n/a	n/a	Heavy Metals: <=0.004%; Melting range 104-108°	55th/R	
420	-	-	66° (1 mm Hg)	IR	98	-	n/a	n/a	Melting point 68-72°	55th/R	
421	insoluble in water	-	[req.]	MS	98	-	n/a	0.5 g/ml at 20°	Melting point 87-93°	55th/R	
426	slightly soluble in water; soluble in ethanol, fat	-	90-100° (15 mm Hg)	IR	99	-	n/a	n/a	Melting point: 88°	55th/R	
433	-	-	142 (5 mmHg)	IR	97	2.0	n/a	n/a	Melting point c.25°	55th/R	
438	soluble in fat, ethanol, propylene glycol and triacetin	-	115 (2 mmHg)	IR	95%	-	1.467-1.473	1.470-1.480	0.973-1.000	55th/R	
439	slightly soluble in water, soluble in alcohols and oils	-	212 (d-isomer)	IR	96	-	1.478 (24°)	0.921		55th/R	
441	-	-	trans 193-196; cis 195-200	MS	98%	-	trans, 1.443 (60°); cis, 1.449 (60°)	n/a		55th/R	
446	soluble in water, olive oil <15% and almond oil 1% w/w	-	n/a	IR	98	0.07	1.4751	1.0308	Congealing point < -10°	55th/R	
451	-	-	170	IR	95%	1.0	1.4868-1.4870 (20°)	1.1351 (20°/20°)		55th/R	
456	slightly soluble in hot water;soluble in hot alcohol, oil	-	199-200	IR	97	-	n/a	n/a	Melting point: 110-112°	55th/R	
458	insoluble in water; miscible in ethyl alcohol and diethyl ether	-	138-139	IR	97	-	1.488-1.492	0.887-0.892		55th/R	
462	soluble in water and fat	-	62-67 (0.35-0.40 mm Hg)	IR, NMR	98	-	1.488-1.498	0.990-0.997		55th/R	
464	insoluble in water; miscible in alcohol and oil	-	89-90 (12mm Hg)	MS	98	-	1.475-1.485	0.970-0.982	80-90% cis isomer	55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
466	3-(Methylthio)propionaldehyde	3-(Methylthio)propionaldehyde	Methional; beta-(Methylmercapto)propionaldehyde, 3-(Methylmercapto)propionaldehyde; beta-Methiopropionaldehyde, beta-(Methylthio)propionaldehyde	2747	125	3268-49-3	104.17	C4 H8 OS	colourless to pale yellow liquid; powerful and diffusive onion and meat-like odour; in dilution, more pleasant, less onion-like, reminiscient of bouillon
467	3-(Methylthio)butanal	3-(Methylthio)butanal	3-(Methylthio)butyraldehyde	3374	11687	16630-52-7	118.19	C5 H10 OS	colourless to pale yellow liquid with green, musky, buchu odour
475	Ethyl 2-(methylthio)acetate	Ethyl (methylthio)acetate	Ethyl beta-(methylthio)propionate	3835		4455-13-4	134.21	C5 H10 O2 S	colourless liquid with a fruity odour
478	3-(Methylthio)propyl acetate	3-(Methylthio)propyl acetate	3-Acetoxypropyl methyl sulfide: Methionyl acetate	3883		16630-55-0	148.22	C6 H12 O2 S	colourless liquid with fatty, estery odour
481	3-(Methylthio)hexyl acetate	3-(Methylthio)hexyl acetate		3789		51755-85-2	190.31	C9 H18 O2 S	colourless liquid
482	S-Methyl thioacetate	S-Methyl acetothioate	Methanethiol acetate, S-Methyl ethanethioate	3876		1534-08-3	90.14	C3 H6 OS	colourless to pale yellow liquid
484	Methyl thiobutyrate	S-Methyl butanethioate	Methylthiol n-butyrate	3310	2328	2432-51-1	118.19	C5 H10 OS	colourless to pale yellow liquid with putrid, rancid, sour, pungent cabbage odour (powerful sweet cheesy odour in dilute solution)
486	S-Methyl 2-methylbutanethioate	S-Methyl 2-methylbutanethioate	Methylthiol 2-methylbutyrate	3708		42075-45-6	132.22	C6 H12 OS	colourless liquid
487	S-Methyl 3-methylbutanethioate	S-Methyl 3-methylbutanethioate	Methylthiol isovalerate	3864		23747-45-7	132.22	C6 H12 OS	colourless liquid
497	4-(Methylthio)-2-butanone	4-(Methylthio)-2-butanone		3375	11688	34047-39-7	118.19	C5 H10 OS	sweet, sulfurous, fruity flavor like arrowhead
498	4,5-Dihydro-3(2H) thiophenone	4,5-Dihydro-3(2H)-thiophenone	Tetrahydrothiophene-3-one; 3-Thiophane	3266	2337	1003-04-9	102.15	C4 H6 OS	colourless to yellow liquid with garlic, meaty, green vegetable, buttery odour
499	2-Methyltetrahydrothiophen-3-one	4,5-Dihydro-2-methyl-3(2H)-thiophenone	2-Methyl-4,5-dihydro-3(2H)thiophenone	3512	11601	13679-85-1	116.18	C5 H8 OS	-
500	4-(Methylthio)-4-methyl-2-pentanone	4-Methyl-4-(methylthio)-2-pentanone		3376	11551	23550-40-5	146.25	C7 H14 OS	-
502	Di(butan-3-one-1-yl) sulfide	Di-(3-oxobutyl) sulfide		3335	11441	40790-04-3	174.26	C8 H14 O2 S	-
503	o-(Methylthio)phenol	2-(Methylthio)phenol	1-Hydroxy-2-methylmercaptobenzene, Methyl (2-hydroxyphenyl) sulfide: 2-Methylmercaptophenol Thioguaiacol	3210	11553	1073-29-6	140.20	C7 H8 OS	liquid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
466	insoluble in water, soluble in alcohol, propylene glycol and oil	1 ml in 1 ml 95% alcohol	165-166	IR	98	10.0	1.479-1.493	1.037-1.052		55th/R	
467	insoluble in water, soluble in alcohol	-	190-192	IR	98	-	1.473-1.517	0.994-1.003		55th/R	
475	very slightly soluble in water, soluble in alcohols and oils	-	70-72 (25 mm Hg)	IR	98	-	1.454-1.462	1.038-1.043		55th/R	
478	very slightly soluble in water, soluble in alcohol and oils	-	201-202	[req.]	97	1.0	1.461-1.467	1.036-1.044		55th/R,T	ID
481	soluble in water and fat	-	75 (5 mm Hg)	IR	99	1.0	1.461-1.469	0.982-0.990		55th/R	
482	soluble in oil and alcohol		95-96	MS, NMR	98		1.460-1.468	0.817-0.825		55th/R	
484	insoluble in water; miscible in diethyl ether	-	140-143, 38-40 (12 mm Hg)	IR	98	1.0	1.457-1.469	0.960-0.975		55th/R	
486	insoluble in water, soluble in fats and alcohols	-	153	MS	99	-	1.456-1.462	1.028-1.035		55th/R	
487	insoluble in water, soluble in peanut oil and ethanol	-	157	IR, MS, NMR, UV	95	-	1.455-1.461	0.935-0.940		55th/R	
497	insoluble in water	-	106 (55 mm Hg); 77-78 (20 mm Hg)	MS	97	-	1.470-1.481	1.000-1.007		55th/R	
498	-	-	174-175, 73 (15 mm Hg), 86-87 (25 mm Hg)	IR	97	-	1.527-1.531	1.194-1.199 (20°)		55th/R	
499	insoluble in water, soluble in alcohol, fats		64-65 (11 mm Hg)	IR	99		1.510-1.520	0.955-0.970		55th/R	
500	-	-	84 (12 mm Hg); 78 (15 mm Hg)	MS	99	-	1.475-1.485	0.964		55th/R	
502	-	-	95 (0.01 mm Hg)	MS	99		[req.]	[req.]		55th/R,T	RI, SG
503	-	-	218-219, 105 (22 mm Hg)	IR	98	-	1.575-1.584	1.168-1.173		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
507	Methylsulfinylmethane	Methylsulfinylmethane	Methyl sulfoxide; Dimethyl sulfoxide (DMSO)	3875		67-68-5	78.13	C_2H_6OS	colourless liquid with mild cabbage or garlic odour
508	Methyl mercaptan	Methenethiol	Methanethiol ; Mercaptomethane; Methyl sulfhydrate; Thiomethyl alcohol	2716	475	74-93-1	48.10	CH_4S	clear liquid (at <6°C) or colourless gas with odour of rotten cabbage or garlic
509	Propanethiol	1-Propanethiol	1-Mercaptopropane; n-Propyl mercaptan	3521	11816	107-03-9	76.16	C_3H_8S	colourless to pale yellow liquid with cabbage-like, sulfuraceous odour
510	2-Propanethiol	2-Propanethiol	Isopropyl mercaptan	3897		75-33-2	76.16	C_3H_8S	colourless liquid with onion odour
512	2-Methyl-1-propanethiol	2-Methyl-1-propanethiol	Isobutyl mercaptan	3874		513-44-0	90.19	$C_4H_{10}S$	colourless liquid with cooked vegetable, mustard-like odour
513	3-Methylbutanethiol	3-Methyl-1-butanethiol	Isoamyl mercaptan	3858		541-31-1	104.22	$C_5H_{12}S$	colourless liquid with odour of onion or glue
514	2-Pentanethiol	2-Pentanethiol	2-Pentyl mercaptan	3792		2084-19-7	104.22	$C_5H_{12}S$	colourless liquid
516	Cyclopentanethiol	Cyclopentanethiol	Cyclopentyl mercaptan	3262	2321	1679-07-8	102.20	$C_5H_{10}S$	colourless liquid
518	1-Hexanethiol	1-Hexanethiol	Hexyl mercaptan	3842		111-31-9	118.24	$C_6H_{14}S$	colourless liquid with earthy odour
520	2, 3, or 10-Mercaptopinane	Mixture of 2,6,6 Trimethyl-bicyclo[3.1.1]heptane-(2, 3 and 10)-thiols	Pinanethiol; Pinanyl mercaptan	3503	2332		170.31	$C_{10}H_{18}S$	sulfurous, tropical fruit, mercaptan odour
521	Allyl mercaptan	Allylthiol	Allyl sulfhydrate	2035	476	870-23-5	74.14	C_3H_6S	colourless to pale yellow mobile liquid with onion-like, sweet, not pungent odour
523	1-p-Menthene-8-thiol	1-p-Menthene-8-thiol	alpha,alpha,4-Trimethyl-3-cyclohexene-1-methanethiol	3700		71159-90-5	170.31	$C_{10}H_{18}S$	Colourless liquid with aroma end taste of grapefruit in dilute solution
524	Thiogeraniol	3,7-Dimethyl-2(trans),6-octadiene-1-thiol	3,7-Dimethyl-2,6-octadien-1-thiol; 3,7-Dimethyl-2,6-octadien-1-yl mercaptan	3472	11583	39067-80-6	170.31	$C_{10}H_{18}S$	yellow to orange liquid
528	o-Toluenethiol	2-Methylbenzenethiol	2-Methyl(thiophenol); o-Tolyl mercaptan	3240	2272	137-06-4	124.20	C_7H_8S	colourless to pale yellow liquid with disagreeable odour
529	2-Ethylthiophenol	2-Ethylbenzenethiol	2-Ethylphenyl mercaptan	3345	11666	4500-58-7	138.23	$C_8H_{10}S$	colourless liquid with disagreeable odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
507	soluble in oil and alcohol, miscible with water	-	189	IR, MS	99	-	1.414-1.420	1.087-1.092		55th/R	
508	2.4 g/100 ml water; soluble in alcohol, ether, organic solvents	-	5.9-6.0	IR	95	1.0	1.430-1.436 (gas); 0.894 (liquid)	0.862-0.894 (gas); 1.032-1.040 (liquid)		55th/R	
509	soluble in water, alcohol, propylene glycol and oils	-	67-68	IR	97	-	1.438	0.842-0.847		55th/R	
510	soluble in oil and alcohol	-	57-60	IR, MS, NMR	98	-	[req.]	0.814-0.819		55th/S,T	RI
512	soluble in oil and alcohol	-	87-89	IR	97	-	1.437-1.444	0.829-0.836		55th/R	
513	soluble in oil and alcohol	-	118-129.5	IR, MS	97	-	1.439-1.447	0.831-0.838		55th/R	
514	slightly soluble in water; soluble in alcohol	-	113	MS	97, +2.4% 3-pentanethiol	-	1.442-1.452	0.832 (d20/4)		55th/R	
516	slightly soluble in water; soluble in alcohol and oils	-	131	MS	98	-	1.488	0.920-0.925		55th/R	
518	soluble in oil and alcohol	-	150-154	IR, MS, NMR	95	-	1.444-1.452	0.824-0.835		55th/R	
520	insoluble in water; soluble in alcohol and oils	-	258-259	IR	95	-	1.511-1.517	0.980-0.988	Contains approx. 54% 10-isomer, 31% 2-isomer, 10% 3-isomer	55th/R	
521	slightly soluble in water; miscible in alcohol, oil, and ethyl ether	1 ml in 1 ml 95% alcohol	66-68	IR	75% (min 98% allyl disulfide + allyl sulfide + allyl mercaptan)	-	1.470-1.491	0.888-0.930		55th/R	
523	slightly soluble in water, soluble in fat	-	37 (0.1 mm Hg); 58 (0.33 mm Hg)	IR	98	-	1.504	0.948 (20°)		55th/R	
524	-	-	58 (0.35 mm Hg)	IR, MS, NMR	95 (+ 5% terpineol)	-	1.503-1.513	0.903-0.921	trans:cis isomer ratio = 6:1	55th/R	
528	-	-	194-195	IR	95	-	1.575	1.054-1.059		55th/R	
529	-	-	203-205	MS	98 (+1-2% 2-ethylphenol)	-	1.568-1.570	1.040-1.045		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
531	2-Naphthalenethiol	2-Naphthalenethiol	2-Mercaptonaphthalene; 2-Naphthyl mercaptan; 2-Thionapthol	3314	2330	91-60-1	160.23	C10 H8 S	crystals with disagreeable mercaptan-like odour
533	bis(Methylthio)methane	Bis(methylthio)methane	2,4-Dithiapentane; Bis(methyl mercapto) methane; Formaldehyde dimethyl dithioacetal; Formaldehyde dimethyl mercaptal; Methylene bis(methyl sulfide); Thioformaldehyde dimethyl acetal	3878		1618-26-4	108.22	C3 H8 S2	pale yellow, oily liquid with an odour of fresh mustard
536	1,2-Propanedithiol	1,2-Propanedithiol	1,2-Dimercaptopropane	3520	11564	814-67-5	108 22	C3 H8 S2	clear blue liquid
544	3-Mercapto-3-methyl-1-butanol	3-Mercapto-3-methyl-1-butanol		3854		34300-94-2	120.20	C5 H 12 OS	-
546	2-Mercapto-3-butanol	3-Mercapto-2-butanol	2-Hydroxy-3-butanethiol; 3-Hydroxy-2-butanethiol	3502	760	37887-04-0	106 18	C4 H10 OS	-
552	Ethyl 2-mercaptopropionate	Ethyl 2-mercaptopropionate	Ethyl thiolactate	3279	11469	19788-49-9	134.19	C5 H10 O2 S	-
558	3-Mercapto-2-butanone	3-Mercapto-2-butanone		3298	11497	40789-98-8	104 17	C4 H8 OS	colourless or pale yellow liquid, becomes cloudy after short storage
560	3-Mercapto-2-pentanone	3-Mercapto-2-pentanone		3300	2327	67633-97-0	118.19	C5 H10 OS	colourless liquid
561	p-Mentha-8-thiol-3-one	8-Mercapto-3-p-menthanone	8-Mercapato-p-menthane-3-one; Thiomenthone	3177	11789	38462-22-5	186.31	C10 H18 OS	colourless to yellow brown liquid
565	Methyl propyl disulfide	Methyl propyl disulfide	Methyl n-propyl disulfide	3201	585	2179-60-4	122.24	C4 H10 S2	pale yellowish mobile liquid with powerful, penetratating, sulfuraceous-herbaceous, oniony odour
572	Allyl disulfide	Diallyl disulfide		2028	485	2179-57-9	146.27	C6 H10 S2	pale yellow liquid with odour of garlic; lacrymator
573	3,5-Dimethyl-1,2,4-trithiolane	3,5-Dimethyl-1,2,4-trithiolane	2,5-Dimethyl-1,3,4-trithiolane; 3,5-Dimethyl-1,2,4-trithiacyclopentane	3541	11883	23654-92-4	152 29	C4 H8 S3	-
574	3-Methyl-1,2,4-trithiane	3-Methyl-1,2,4-trithiane	3-Methyl-1,2,4-trithiacyclohexane	3718		43040-01-3	152.29	C4 H8 S3	colourless liquid with strong odour
575	Dicyclohexyl disulfide	Dicyclohexyl disulfide		3448	2320	2550-40-5	230.43	C12 H22 S2	-

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
531	slightly soluble in water; soluble in alcohol and ether	-	210.5 (100mm Hg)	MS	98	-	n/a	1.160 (d20/4)	Melting point 81°C; Decomposes at 285°C	55th/R	
533	very slightly soluble in water; soluble in alcohols and oils	-	193	IR	99	-	1.530-1.538	0.959-1.059		55th/R	
536	insoluble in water, miscible in oil	-	152	IR, NMR	96	-	1.531-1.541	1.075-1.081	Chlorinated monothiol: max. 1.1%	55th/R	
544	soluble in water at 10 g/l at 20°C, white petrolatum at <100 g/kg at 20°C, acetone and 95% ethanol at 20°C	-	186 (730 mm Hg)	IR, MS, NMR	96	-	1.480-1.490	0.989 (20°)		55th/R	
546	insoluble in water; miscible in alcohol and fat	-	58-60 (10 mm Hg)	IR, NMR	99	-	1.476-1.485	1.010-1.017		55th/R	
552	-	-	40-41 (1 mm Hg)	IR	99	-	1.447-1.452	1.027-1.050		55th/R	
558	slightly soluble in water; soluble in alcohol, ether, pyridine and aqueous alkalis	-	50 (18 mm Hg)	IR	99	-	1.469-1.479	1.016 (20°)		55th/R	
560	insoluble in water, miscible in alcohol	-	183; 57 (15 mm Hg)	MS	98	-	1.414-1.424	0.988-0.998		55th/R	
561	insoluble in water soluble in alcohol	-	120 (10 mm Hg)	IR	97	-	1.492-1.509	0.995-1.010		55th/R	
565	slightly soluble in water; soluble in ethyl alcohol and oil	-	69-71 (43 mm Hg); 40-41 (9 mm Hg)	MS	95	-	1.508-1.518	0.990-0.999		55th/R	
572	insoluble in water; soluble in common organic solvents	-	79 (16 mm Hg)	IR	80 (min. 95% allyl disulfide + allyl sulfide + allyl mercaptan)	-	1.537-1.551	0.998-1.015		55th/R	
573	insoluble in water; soluble in fat	-	43-45 (0.7 mm Hg)	IR	98	-	1.593-1.603	1.241-1.261		55th/R	
574	insoluble in water; soluble in fat	-	226	MS	98	-	1.617-1.627	1.276 (d20/4)		55th/R	
575	insoluble in water; slightly soluble in alcohol; soluble in fat	-	162-163 (6 mm Hg)	NMR	97	-	1.543-1.553	1.042-1.049		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
579	Benzyl disulfide	Dibenzyl disulfide	BDS; alpha-(Benzyldithio))toluene; 1,4-Diphenyl-1,2,3-dithiobutane, Di(phenylmethyl)disulfide	3617		150-60-7	246.39	C14 H14 S2	pale yellowish leafy crystals or leaflets with "burnt caramellic" odour
582	Dimethyl trisulfide	Dimethyl trisulfide		3275	539	3658-80-8	126.26	C2 H6 S3	pale yellow liquid with powerful odour
584	Methyl propyl trisulfide	Methyl propyl trisulfide		3308	586	17619-36-2	154.30	C4 H10 S3	Pale yellow, mobile liquid with powerful, penetrating, warm, herbaceous odour somewhat reminiscent of onion
585	Dipropyl trisulfide	Dipropyl trisulfide		3276	726	6028-61-1	182.36	C6 H14 S3	colourless liquid with powerful, diffusive garlic-like odour
587	Diallyl trisulfide	Diallyl trisulfide	Allyl trisulfide	3265	486	2050-87-5	178.33	C6 H10 S3	yellow liquid with disagreeable odour
588	Diallyl polysulfide	Mixture of diallyl di-, tri-, tetra-, and pentasulfides	2-Propenyl polysulfides	3533	11912	72869-75-1		C6 H10 Sx (x=2-5)	pale yellow liquid with strong garlic-like odour
589	2-Oxobutyric acid	2-Oxobutyric acid	alpha-Ketobutyric acid	3723		600-18-0	102.09	C4 H6 O3	-
592	Citronelloxyacetaldehyde	6,10-Dimethyl-3-oxa-9-undecenal	6,10-Dimethyl-3-oxa-9-undecenal	2310	2012	7492-67-3	198.31	C12 H22 O2	colourless viscous liquid with strong floral odour
594	Ethyl 3-Hydroxybutyrate	Ethyl 3-hydroxybutyrate	Ethyl 3-hydroxybutanoate	3428	10596	5405-41-4	132.16	C6 H12 O3	colourless viscous liquid with fruity grape green odour
596	Butyl acetoacetate	Butyl 3-oxobutyrate	Butyl 3-ketobutanoate; Butyl beta-ketobutanoate; Butyl beta-ketobutyrate; Butyl 3-oxobutanoate	2176	241	591-60-6	158.20	C8 H14 O3	colourless liquid; fruity taste; sweet, brandy-like odour of fermented fruit
597	Isobutyl acetoacetate	2-Methylpropyl 3-oxobutyrate	iso-Butyl acetoacetate; iso-Butyl beta-ketobutyrate; iso-Butyl 3-oxobutanoate; Isobutyl beta-ketobutyrate; Isobutyl 3-oxobutanoate	2177	242	7779-75-1	158.20	C8 H14 O3	colourless liquid; fruity taste; sweet, fruity odour of brandy
598	Isoamyl acetoacetate	3-Methylbutyl 3-oxobutyrate	iso-Amyl acetoacetate; iso-Amyl beta-ketobutyrate; iso-Amyl 3-oxobutanoate; Isobutyl beta-ketobutyrate, Isobutyl 3-oxobutanoate	3551	227	2308-18-1	172.23	C9 H16 O3	colourless liquid, ethereal, fruity, somewhat herbaceous, winey, fermented apple-like odour
600	Methyl 3-hydroxyhexanoate	Methyl 3-hydroxyhexanoate	Methyl 3-hdroxycaproate, Methyl beta-hydroxycaproate; Methyl beta-hydroxyhexanoate	3508	10812	21188-58-9	146.19	C7 H14 O3	colourless to pale yellow liquid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
579	insoluble or slightly soluble in water; soluble in hot alcohol, ether	-	>270 (with decomposition)	IR	98	-	n/a	n/a	Melting point 71-74°	55th/R	
582	very slightly soluble in water; soluble in alcohols, propylene glycol and oils	-	165-170; 41 (6 mm Hg)	IR	97	-	1.595-1.605	1.195-1.210		55th/R	
584	-	-	52 (1.2 mm Hg)	IR	45	-	1.558-1.570	1.095-1.101	Also contains min. 25% dipropyl trisulfide, 12% dipropyl disulfide, 14% dimethyl disulfide, 3% methyl propyl sulfide	55th/R	
585	almost insoluble in water; soluble in alcohol and oils	-	98 (4mm Hg); 93 (6 mm Hg), 86-89 (1.5 mm Hg)	IR	99 (including up to 15% dipropyl disulfide)	-	1.542-1.590	0.952		55th/R	
587	insoluble in water and alcohol; miscible with ether	-	112-120 (16 mm Hg) 95-97 (5 mm Hg); 70 (1.0 mm Hg)	IR	65 (min. 95% allyl di-, tri- and tetra-sulfides)	-	1.600-1.620	1.135-1.170		55th/R	
588	insoluble in water; slightly soluble in alcohol; miscible in oil	-	68 (15 mm Hg)	IR, NMR	95	-	1.643-1.653	1.220 (20°)	allyl disulfides 2-10%; allyl trisulfides 20-30%; allyl tetrasulfides 30-40%; allyl pentasulfides 30-40%	55th/R	
589	soluble in water and alcohol	-	80-82 (16 mm Hg)	IR	98	-	n/a	1.200 (d20/4)	Melting point 31-32°	55th/R	
592	insoluble in water; soluble in alcohol	-	239; 130 (12 mm Hg)	MS	75	-	1.461-1.471	0.922 (20°)		55th/R,T	Low assay
594	100 g in 100 ml water at 23°C	-	170; 67 (4 mm Hg)	MS	99	-	1.416-1.424	1.010-1.017		55th/R	
596	Insoluble in water; soluble in alcohol and oil	-	205;100-103 (16 mm Hg)	MS	97	-	1.425-1.435	0.976		55th/R	
597	insoluble in water; soluble in alcohol and oil	-	196; 84.5 (11 mm Hg)	IR	98	-	1.422-1.432	0.970		55th/R	
598	insoluble in water; soluble in alcohol	-	222-224	IR	97	-	1.426-1.433	0.954 (10°)		55th/R	
600	insoluble in water and fat	-	65 (2 mm Hg)	IR	95	-	1.410-1.440	0.994-1.010		55th/R	

No	Name	Chemical name	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
604	3-(Hydroxymethyl)-2-heptanone	3-(Hydroxymethyl)-2-heptanone	2-Acetyl-1-hexanol; Methylol methyl amyl ketone	2804	592	65405-68-7	144.21	C8 H16 O2	colourless liquid with powerful, herbaceous, fruity, mildly spicy odour
605	1,3-Nonanediol acetate (mixed esters)	Mixture of 3-Acetoxynonyl acetate, 3-Hydroxynonyl acetate and 1-(2-Hydroxyethyl)heptyl acetate	Diasmol; 3-Hexyl-1,3-propanediol acetate, mixed esters, Nonane diacetate	2783	2075	1322-17-4		C11 H22 O3	colourless to pale yellow, slightly oily liquid with floral odour similar to jasmine
610	Hydroxycitronellol	2,6-Dimethyl-2,8-octanediol	Citronellol hydrate	2586	559	107-74-4	174.29	C10 H22 O2	colourless very viscous liquid; mild sweet odour
613	Hydroxycitronellal diethyl acetal	8,8-Diethoxy-2,6-dimethyl-2-octanol	1,1-Diethoxy-3,7-dimethyl-7-octanol	2584	44	7779-94-4	246.39	C14 H30 O3	colourless slightly oily liquid; delicate green floral taste
618	Fumaric acid	2(trans)-Butenedioic acid	Allomaleic acid, Boletic acid; (E)-Butenedioic acid; (E)-1,2-Ethylenedicarboxylic acid	2488	25	110-17-8	116.07	C4 H4 O4	white odourless granules or leafy crystals; virtually odourless with tart acid taste
619	l-Malic acid	2-Hydroxybutanedioic acid	2-Hydroxybutanedioic acid; Hydroxysuccinic acid	2655	17	97-67-6	134.09	C4 H6 O5	white crystalline powder, granules, or needles; acid taste; odourless or having a very faint caramellic acrid odour and a tart aciduous taste
620	Diethyl malate	Diethyl 2-hydroxybutanedioate	Diethyl 2-hydroxybutanedioate; Diethyl hydroxysuccinate; Ethyl malate; dl-Ethyl malate	2374	382	7554-12-3	190.20	C8 H14 O5	colourless liquid; mild, winey-fruity odour with pleasant herbaceous undertone
629	Triethyl citrate	Triethyl 2-hydroxy-1,2,3-propanetricarboxylate	Ethyl citrate; Triethyl 2-hydroxy-1,2,3-propane-tricarboxylate	3083	11762	77-93-0	276.29	C12 H20 O7	practically colourless, oily liquid; bitter taste; little odour
630	Tributyl acetylcitrate	Tributyl 2-acetoxy-1,2,3-propanetricarboxylate	Acetyl tributyl citrate	3080		77-90-7	402.48	C20 H34 O8	colourless, slightly viscous liquid with very faint sweet herbaceous odour
631.1	3-Methyl-2-oxobutanoic acid, sodium salt	Sodium 3-methyl-2-oxobutyrate	Sodium, alpha-ketoisovalerate; Butanoic acid, 3-methyl-2-oxo-, sodium salt; Sodium 3-methyl-2-oxobutanoate	3869		3715-29-6	138.10	C5 H7 O3 Na	-
632.1	3-Methyl-2-oxopentanoic acid, sodium salt	Sodium 3-methyl-2-oxovalerate	Valeric acid, 3-methyl-2-oxo-, sodium salt	3870		3715-31-9	152.10	C6 H9 O3 Na	-
633.1	4-Methyl-2-oxopentanoic acid, sodium salt	Sodium 4-methyl-2-oxovalerate	Valeric acid, 4-methyl-2-oxo, sodium salt, Sodium 4-methyl-2-ketopentanoate; Sodium 4-methyl-2-oxopentanoate	3871		4502-00-5	152.10	C6 H9 O3 Na	-

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
604	slightly soluble in water; soluble in alcohol	-	94.6 (8-9 mm Hg)	MS	90	-	1.444-1.447	0.945-0.949		55th/R,T	Low assay
605	slightly soluble in water; soluble in alcohol and oils	1 ml in 1 ml 95% alcohol	200-255	IR	95 (total of 2 monoesters and diester)	1 0	1.441-1.453	0.964-0.978		55th/R,T	BP
610	slightly soluble in water; soluble in alcohol and oils	1 ml in 1 ml 60% alcohol	263; 156 (15 mm Hg)	IR	97	-	1.455-1.460	0.922-0.930	Aldehyde content max. 10% (as hydroxycitronellal)	55th/R	
613	insoluble in water; soluble in alcohol and oil	-	260; 135 (3 mm Hg)	IR	95	-	1.435-1.440	0.902-0.908		55th/R	
618	insoluble to slightly soluble in water; soluble in alcohol, slightly soluble in oils	-	n/a	MS	99 5	-	n/a	n/a	Heavy Metals: max. 10 ppm; Maleic acid: max 0.1%; Water: max. 0.5%; Residue on Ignition: max 0.1%; sublimes at 200°	55th/R	
619	soluble in water and alcohol; 1 gm in 0.8 ml water	1 g in 1.4 ml alcohol	n/a	IR	99	-	n/a	n/a	Melting point. 100°; Fumaric Acid: max. 1.0%; Heavy Metals: max 10 ppm; Maleic acid. max. 0.05%; Residue on Ignition: max 0.1 %; Specific Rotation: -0.23° at 25°; Water Insoluble Matter: max. 0.1%	55th/R	
620	soluble in water; miscible in alcohol and oil	-	254, 91-92 (1 mm Hg)	MS	99	-	1.436-1.446	1.120-1.128		55th/R	
629	slightly soluble in water; miscible with alcohol and ether	-	294	IR	99	-	1.440-1.444	1.138-1.139	Acidity: max 0.02% as citric acid; Heavy Metals; max. 10 ppm; Water: max. 0.25%	55th/R	
630	insoluble in water; soulble in alcohol; miscible in oil	-	172-174 (1 mm Hg)	IR	99	0.02%	1.440-1.445	1.140; 1.045-1.055		55th/R	
631.1	-	-	n/a	NMR	95% by non-aqueous titration	-	n/a	n/a		55th/R,T	A(m)
632.1	-	-	n/a	NMR	96% by HPLC	-	n/a	n/a		55th/R,T	A(m)
633.1	-	-	n/a	NMR	98% by non-aqueous titration	-	n/a	n/a		55th/R,T	A(m)

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
450	Furfural	2-Furfuraldehyde	2-Formylfuran; Fural; 2-Furaldehyde; Furfuraldehyde; 2-Furylcarboxaldehyde; Pyromucic aldehyde	2489	2014	98-01-1	96.09	C5 H4 O2	Colourless to yellow oily liquid which browns on storage, pungent, sweet, bread-like, caramellic, cinnamon-almond-like flavour, odour resembles benzaldehyde
451	Furfuryl alcohol	Furfuryl alcohol	2- Furancarbinol; Furfuralcohol; alpha-Furylcarbinol; 2-Hydroxymethylfuran	2491	2023	98-00-0	98.10	C5 H6 O2	Colourless or pale yellowish liquid, mild, warm oily, "burnt" odour
636	3-Phenyl-1-propanol	3-Phenylpropanol	Hydrocinnamyl alcohol; Phenethyl carbinol; 3-Hydroxy-1-phenylpropane; (3-Hydroxypropyl)benzene	2885	80	122-97-4	136.19	C9 H12 O	Colourless, slightly viscous liquid, sweet hyacinth odour
637	3-Phenylpropyl formate	Benzenepropanol formate	Hydrocinnamyl formate; beta-Phenylpropyl formate	2895	351	104-64-3	164.20	C10 H12 O2	Colourless to slightly yellow liquid, pleasant, sweet, floral-herbaceous odour
638	3-Phenylpropyl acetate	Benzenepropanol acetate	Hydrocinnamyl acetate; beta-Phenylpropyl acetate	2890	222	122-72-5	178.23	C11 H14 O2	Colourless liquid, floral spicy odour
639	3-Phenylpropyl propionate	Benzenepropanol propionate	Hydrocinnamyl propionate; beta-Phenylpropyl propionate	2897	419	122-74-7	192.26	C12 H16 O2	Colourless liquid, heavy floral balsamic odour
640	3-Phenylpropyl isobutyrate	3-Phenylpropyl isobuyrate	Hydrocinnamyl isobutyrate; 3-Phenylpropyl 2-methylpropanoate; beta-Phenylpropyl-2-methylpropanoate	2893	303	103-58-2	206.28	C13 H18 O2	Colourless liquid, fruity-balsamic sweet odour
641	3-Phenylpropyl isovalerate	3-Phenylpropyl isovalerate	Hydrocinnamyl isovalerate; 3-Phenylpropyl isopentanoate; beta-Phenylpropyl 3-methylbutanoate	2899	462	5452-07-3	220.31	C14 H20 O2	Colourless liquid, strawberry-prune-plum-like odour
642	3-Phenylpropyl hexanoate	3-Phenylpropyl hexanoate	Hydrocinnamyl caproate; 3-Phenylpropyl caproate	2896	321	6281-40-9	234.34	C15 H22 O2	Colourless liquid, sweet, fruity-green odour
643	Methyl 3-phenylpropionate	Methyl 3-phenylpropionate	Methyl hydrocinnamate	2741	427	103-25-3	164.20	C10 H12 O2	Colourless liquid, powerful, fruity-winey floral sweet odour
644	Ethyl 3-phenylpropionate	Ethyl 3-phenylpropionate	Ethyl hydrocinnamate	2455	429	2021-28-5	178.23	C11 H14 O2	Colourless, somewhat oily liquid, sweet, fruity, honey-like odour
645	3-Phenylpropionaldehyde	Benzenepropanel	Benzylacetaldehyde; Hydrocinnamaldehyde; Phenylpropyl aldehyde	2887	2013	104-53-0	134.18	C9 H10 O	Colourless to slightly yellow liquid, strong pungent floral odour of hyacinth
646	3-Phenylpropionic acid	Benzenepropanoic acid	Benzylacetic acid; Hydrocinnamic acid; beta-Phenylpropionic acid	2889	32	501-52-0	150.18	C9 H10 O2	White crystalline solid, faint, sweet, somewhat balsamic and coumarin-like odour
647	Cinnamyl alcohol	Cinnamyl alcohol	Cinnamic alcohol; gamma-Phenylallyl alcohol; Zimtalcohol	2294	65	104-54-1	134.18	C9 H10 O	White to yellowish crystalline solid, warm-balsamic, floral, sweet odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
450	soluble in water; soluble in oils	miscible	161-162	IR	95	3.0	1.521-1.529	1.153-1.162		55th/R	-
451	miscible in water; miscible in oils	miscible	169-171	IR	97	-	1.481-1.489	1.126-1.136		55th/R	-
636	slightly soluble in water; soluble in oils	miscible	235-236	IR	98	1.0	1.524-1.528	0.993-1.002		55th/N	-
637	insoluble in water	miscible	238	MS	97	1.0	1.494-1.499	1.012-1.019		55th/N	-
638	insoluble in water; soluble in oils	miscible	244-245	IR	98	1.0	1.494-1.498	1.011-1.020		55th/N	-
639	insoluble in water; soluble in oils	miscible	265	MS	99	1.0	1.488-1.495	0.995-1.005		55th/N	-
640	insoluble in water; soluble in oils	miscible	258	IR	98	1.0	1.483-1.493	0.975-0.981		55th/N	-
641	insoluble in water; soluble in oils	miscible	280	IR	93	1.0	1.482-1.489	0.962-0.971		55th/N	-
642	insoluble in water; soluble in oils	miscible	292	[req.]	99	1.0	[req.]	0.963-1.010		55th/N,T	ID, RI
643	insoluble in water	miscible	238-239	IR	98	1.0	1.499-1.505	1.037-1.045		55th/N	-
644	insoluble in water; soluble in oils	miscible	247-249°	IR	98	1.0	1.492-1.497	1.009-1.017		55th/N	-
645	insoluble in water; soluble in oils	miscible	222	IR	90 by aldehyde determination	5.0	1.518-1.528	1.008-1.018		55th/N,T	A(e): Low assay
646	slightly soluble in water; soluble in oils	moderately soluble	280	IR	97; 98 by titration	-	n/a	n/a	mp: 43° minimum	55th/N	-
647	insoluble to slightly soluble in water; soluble in oils	moderately soluble	258	IR	98	-	n/a	n/a	mp: 30° minimum	55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
648	Cinnamaldehyde ethylene glycol acetal	2-Styryl-1,3-dioxolane	Cincloval; 2-Styryl-1,3-dioxolane	2287	48	5660-60-6	176.22	$C_{11}H_{12}O_{2}$	Nearly colourless oily liquid, soft, spicy, warm, sweet odour
649	Cinnamyl formate	Cinnamyl formate	3-Phenylallyl formate	2299	352	104-65-4	162.19	$C_{10}H_{10}O_{2}$	Colourless to slightly yellow liquid, green, herbaceous, balsamic odour
650	Cinnamyl acetate	Cinnamyl acetate	3-Phenylallyl acetate	2293	208	103-54-8	176.22	$C_{11}H_{12}O_{2}$	Colourless to slightly yellow liquid, sweet, balsamic, floral odour
651	Cinnamyl propionate	Cinnamyl propionate	3-Phenylallyl propionate	2301	414	103-56-0	190.24	$C_{12}H_{14}O_{2}$	Colourless to pale yellow liquid, fruity-floral odour
652	Cinnamyl butyrate	Cinnamyl butyrate	3-Phenylallyl butyrate	2296	279	103-61-7	204.27	$C_{13}H_{16}O_{2}$	Colourless to yellowish liquid, fruity slightly floral balsamic odour
653	Cinnamyl isobutyrate	Cinnamyl isobutyrate	Cinnamyl 2-methylpropanoate; 3-Phenyl-2-propen-1-yl isobutyrate	2297	496	103-59-3	204.27	$C_{13}H_{16}O_{2}$	Colourless to yellowish liquid, sweet, balsamic fruity odour
654	Cinnamyl isovalerate	Cinnamyl isovalerate	Cinnamyl 3-methyl butanoate; 3-Phenylallyl isovalerate; 3-Phenylallyl 3-methylbutanoate	2302	454	140-27-2	218.30	$C_{14}H_{18}O_{2}$	Colourless to pale yellow liquid, spicy, fruity, floral odour
655	Cinnamyl phenylacetate	Cinnamyl phenylacetate	Cinnamyl alpha-toluate; 3-Phenylallyl phenylacetate	2300	235	7492-65-1	252.31	$C_{17}H_{16}O_{2}$	Colourless, slightly viscous liquid, deep chrysanthemum-like odour
656	Cinnamaldehyde	3-Phenyl-2-propenal	Cinnamal; Cinnamic aldehyde; beta-Phenylacrolein; Zimtaldehyde, Cassia aldehyde; Benzylidene acetaldehyde	2286	102	104-55-2	132.16	$C_{9}H_{8}O$	Yellow liquid, strong cinnamon odour
657	Cinnamic acid	3-Phenyl-2-propenoic acid	Benzene propenoic acid; Benzyldeneacetic acid; 3-Phenylacrylic acid; beta-Phenylacrylic acid	2288	22	621-82-9	148.16	$C_{9}H_{8}O_{2}$	White crystalline scales, honey floral odour
658	Methyl cinnamate	Methyl cinnamate		2698	333	103-26-4	162.19	$C_{10}H_{10}O_{2}$	Colourless crystalline mass, fruity balsamic odour
659	Ethyl cinnamate	Ethyl cinnamate	Ethyl phenylacrylate	2430	323	103-36-6	176.22	$C_{11}H_{12}O_{2}$	Colourless liquid, sweet balsamic-honey note
660	Propyl cinnamate	Propyl cinnamate	Propyl beta-phenylacrylate	2938	324	7778-83-8	190.24	$C_{12}H_{14}O_{2}$	Colourless viscous liquid, sweet, slightly floral odour
661	Isopropyl cinnamate	Isopropyl cinnamate	1-Methylethyl 3-phenylpropenoate	2939	325	7780-06-5	190.24	$C_{12}H_{14}O_{2}$	Colourless viscous liquid, balsamic, sweet and dry amber type odour
663	Butyl cinnamate	Butyl cinnamate	Butyl beta-phenylacrylate	2192	326	538-65-8	204.27	$C_{13}H_{16}O_{2}$	Colourless, oily, somewhat viscous liquid, sweet, oily, balsamic, fruity odour
664	Isobutyl cinnamate	Isobutyl cinnamate	Isobutyl beta-phenylacrylate; Labdanol; 2-Methylpropyl cinnamate; 2-Methylpropyl beta-phenylacrylate	2193	327	122-67-8	204.27	$C_{13}H_{16}O_{2}$	Colourless liquid, sweet fruity balsamic odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
648	insoluble in water; soluble in oils	miscible	265	(req.)	90	-	1.561-1.570	1.095-1.103		55th/N,T	ID
649	insoluble in water; soluble in oils	miscible	250	IR	95	3.0	1.550-1.556	1.075-1.082		55th/N	-
650	insoluble in water; soluble in oils	miscible	262-265	IR	98	3.0	1.539-1.544	1.047-1.054		55th/N	-
651	insoluble in water	miscible	289	IR	98	3.0	1.532-1.537	1.029-1.034		55th/N	-
652	insoluble in water	miscible	300	(req.)	98	1.0	1.525-1.530	1.010-1.020		55th/N,T	ID
653	insoluble in water; soluble in oils	miscible	254	IR	96	3.0	1.520-1.528	1.005-1.014		55th/N	-
654	insoluble in water; miscible in oils	miscible	313	IR	95	3.0	1.517-1.524	0.990-0.996		55th/N	-
655	insoluble in water	miscible	333-335	IR	96	1.0	1.575-1.581	1.089-1.095		55th/N	-
656	insoluble in water; miscible in oils	miscible	248-250	IR	98 by aldehyde determination	10.0	1.619-1.625	1.046-1.053		55th/N,T	A(e)
657	insoluble in water; soluble in oils	slightly soluble	300	IR	98 by titration	-	n/a	n/a	mp: 132° minimum	55th/N	-
658	insoluble in water; soluble in oils	moderately soluble	262-263	IR	98	2.0	n/a	n/a	mp: 33° minimum	55th/N	-
659	insoluble in water; miscible in alcohols	miscible	271-272	IR	99	1.0	1.558-1.562	1.044-1.051		55th/N	-
660	insoluble in water; soluble in oils	miscible	283-284	IR	98 by ester determination	1.0	1.547-1.553	1.030-1.040		55th/N,T	A(e)
661	insoluble in water; soluble in oils	miscible	268-270	MS	98	1.0	1.541-1.548	1.020-1.027		55th/N	-
663	slightly soluble to insoluble in water	miscible	287	IR	98 by ester determination	1.0	1.539-1.545	1.008-1.014		55th/N,T	A(e)
664	insoluble in water; soluble in oils	miscible	287	IR	97	1.0	1.538-1.542	1.001-1.005		55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
665	Isoamyl cinnamate	Isopentyl cinnamate	Isoamyl beta-phenylacrylate, Isopentyl cinnamate	2063	335	7779-65-9	218.30	C14 H18 O2	Colourless to slightly yellow liquid with a balsamic odour
666	Heptyl cinnamate	Heptyl cinnamate	Heptyl beta-phenylacrylate	2551	2104	10032-08-3	246.35	C16 H22 O2	Colourless or pale-straw coloured viscous liquid, mild, floral-green, somewhat bark-like odour
667	Cyclohexyl cinnamate	Cyclohexyl cinnamate	Cyclohexyl beta-phenylacrylate	2352	337	7779-17-1	230.31	C15 H18 O2	Colourless to light yellow liquid, fruit, peach, cherry, almond like odour
668	Linalyl cinnamate	Linalyl cinnamate	3,7-Dimethyl-1,6-octadien-3-yl cinnamate; 3,7-Dimethyl-1,6-octadien-3-yl beta-phenylacrylate; 3,7-Dimethyl-1,6-octadien-3-yl 3-phenylpropenoate	2641	329	78-37-5	284.40	C19 H24 O2	Almost colourless, oily, somewhat viscous liquid, mild, balsamic, sweet, slightly herbaceous, floral odour
669	Terpinyl cinnamate	(Z)-1-Methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl cinnamate	p-Menthen-1-en-8-yl cinnamate; Terpinyl beta-phenylacrylate; Terpinyl 3-phenylpropenoate	3051	330	10024-56-3	284.40	C19 H24 O2	Colourless or pale straw coloured viscous liquid, mild, sweet, floral-balsamic odour
670	Benzyl cinnamate	Benzyl cinnamate	Benzyl beta-phenylacrylate, Cinnamein	2142	331	103-41-3	238.29	C16 H14 O2	White to pale yellow solid
671	Phenethyl cinnamate	Phenyethyl cinnamate	Benzylcarbinyl cinnamate; Benzylcarbinyl 3-phenylpropenoate; beta-Phenethyl beta-phenylacrylate; 2-Phenylethyl cinnamate	2863	336	103-53-7	252.31	C17 H16 O2	White crystals, heavy balsamic-like rosy odour
672	3-Phenylpropyl cinnamate	3-Phenylpropyl cinnamate	Hydrocinnamyl cinnamate; Hydrocinnamyl 3-phenylpropenoate; beta-Phenylpropyl cinnamate; 3-Phenylpropyl beta-phenylacrylate	2894	338	122-68-9	266.34	C18 H18 O2	Colourless to slightly yellow liquid, rosy balsamic delicately fruity odour
673	Cinnamyl cinnamate	Cinnamyl cinnamate	Cinnamyl beta-phenylacrylate; 3-Phenylallyl cinnamate; Phenylallyl cinnamate	2298	332	122-69-0	264.32	C18 H16 O2	White or colourless crystals, mild, balsamic, floral odour
674	alpha-Amylcinnamyl alcohol	2-Pentyl-3-phenylprop-2-en-1-ol	n-Amylcinnamic alcohol; 2-Benzylideneheptanol; alpha-Pentylcinnamyl alcohol	2065	79	101-85-9	204.31	C14 H20 O	Colourless to slightly yellow liquid, light floral note
675	5-Phenylpentanol	Benzenepentan-1-ol	Phenylamyl alcohol	3618	674	10521-91-2	164 25	C11 H16 O	Colourless liquid, floral carnation note
676	alpha-Amylcinnamyl formate	2-(Phenylmethylene)heptyl formate	alpha-Amyl-beta-phenylacryl formate; alpha-Pentylcinnamyl formate	2066	357	7493-79-0	232.32	C15 H20 O2	Colourless liquid, sweet, oily herbaceous, and somewhat green odour
677	alpha-Amylcinnamyl acetate	2-(Phenylmethylene)heptyl acetate	alpha-n-Amyl-beta-phenylacryl acetate; alpha-Pentylcinnamyl acetate	2064	216	7493-78-9	246.35	C16 H22 O2	Colourless oily liquid, mild, oily, fruity, somewhat green odour
678	alpha-Amylcinnamyl isovalerate	2-(Phenylmethylene)heptyl isovalerate	alpha-Amyl-beta-phenylacryl isovalerate; alpha-n-Amyl-beta-phenylacryl 3-methylbutanoate; alpha-Pentylcinnamyl isovalerate	2067	463	7493-80-3	288.43	C19 H28 O2	Colourless liquid, mild fruity, somewhat herbaceous tobacco-like odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
665	insoluble in water; soluble in oils	miscible	310	IR	97	1.0	1.533-1.541	0.992-0.997		55th/N	-
666	insoluble in water; soluble in oils	miscible	185 (12 mm Hg)	[req.]	97	1.0	1.528-1.530	0.982-0.990		55th/N,T	ID
667	insoluble in water	miscible	195 (12 mm Hg)	MS	95	1.0	1.558-1.564	1.047-1.056		55th/N	-
668	insoluble in water	miscible	353	IR	94	6.0	1.540-1.545	0.985-0.995		55th/N,T	Low assay
669	insoluble in water; miscible in oils	miscible	360	[req.]	[req.]	1.0	1.548-1.552	[req.]		55th/N,T	ID, A, SG
670	insoluble in water; soluble in oils	very soluble	350, 195 (5 mm Hg)	IR	98	1.0	n/a	n/a	solidifies at 25° (minimum)	55th/N	-
671	insoluble in water; soluble in oils	moderately soluble	[req.]	IR	98	1.0	n/a	n/a	mp: 54° (minimum)	55th/N,T	BP
672	insoluble in water; soluble in oils	miscible	190 (0.2 mm Hg)	IR	98 by ester determination	1.0	1.583-1.588	1.074-1.080		55th/N,T	A(e)
673	insoluble in water; soluble in oils	moderately soluble	370	IR	95 by ester determination	2.0	n/a	n/a	mp: 42° (minimum)	55th/N,T	A(e)
674	insoluble in water	miscible	141 (5 mm Hg)	IR	95	-	1.533-1.540	0.954-0.962		55th/N	-
675	insoluble in water; soluble in oils	miscible	155 (20 mm Hg)	IR	98	5.0	1.514-1.521	0.970-0.977		55th/N	-
676		miscible	[req.]	[req.]	[req.]	-	[req.]	[req.]		55th/N,T	BP, ID, A, RI, SG
677	soluble in oils	miscible	[req.]	[req.]	97	1.0	1.487-1.495	0.953-0.961		55th/N,T	BP, ID
678		miscible	[req.]	[req.]	[req.]	-	[req.]	[req.]		55th/N,T	BP, ID, A, RI, SG

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
679	3-Phenyl-4-pentenal	3-Phenylpent-4-enal	3-Phenyl-3-vinylpropionaldehyde; beta-Vinylhydrocinnamaldehyde	3318	10378	939-21-9	160.22	C11 H12 O	
680	3-(p-Isopropylphenyl) propionaldehyde	3-(p-Cumenyl)propionaldehyde	Cuminylacetaldehyde, p-Cuminylpropanal; p-Isopropylhydrocinnamaldehyde ; 3-(p-Cumenyl)propionaldehyde	2957	2261	7775-00-0	176.26	C12 H16 O	Colourless to pale yellow liquid, strong floral odour
681	alpha-Amylcinnamaldehyde dimethyl acetal	(2-(Dimethoxymethyl)-1-heptenyl)benzene	alpha-Amyl-beta-phenylacrolein dimethyl acetal; 1,1-Dimethoxy-2-benzylideneheptane. alpha-Pentylcinnamaldehyde dimethyl acetal; alpha-Amylcinnamic aldehyde dimethyl acetal	2062	47	91-87-2	248.36	C16 H24 O2	Almost colourless to pale yellow, floral odour reminiscent of jasmine
682	p-Methylcinnamaldehyde	2-Propenal, 3-(4-methylphenyl)-	3-(p-Methylphenyl) propenal; 3-p-Tolylpropenal	3640	10352	1504-75-2	146.19	C10 H10 O	Yellowish crystals
683	alpha-Methylcinnamaldehyde	alpha-Methylcinnamaldehyde	alpha-Methylcinnamic aldehyde; 3-Phenyl-2-methylacrolein; alpha-Methylcinnamyl aldehyde;	2697	578	101-39-3	146.19	C10 H10 O	Yellow liquid, cinnamon-like odour
684	alpha-Butylcinnamaldehyde	alpha-Butylcinnamaldehyde	2-Benzylidenehexanal; Butylcinnamic aldehyde; alpha-Butyl-beta-phenylacrolein	2191	127	7492-44-6	188.27	C13 H16 O	Pale yellowish oily liquid, green-oily-herbaceous odour
685	alpha-Amylcinnamaldehyde	alpha-Pentylcinnamaldehyde	"A C.A.": Amyl cinnamal, alpha-Amyl-beta-phenylacrolein; Buxine; Flomine; Flosal; Floxine; Jasmine aldehyde; Jasmonal; alpha-Pentylcinnamaldehyde	2061	128	122-40-7	202.30	C14 H18 O	Pale yellowish liquid. strong floral odour suggestive of jasmine
686	alpha-Hexylcinnamaldehyde	alpha-Hexylcinnamaldehyde	2-Benzylideneoctanal; "H.C.A."; alpha-n-Hexylcinnamic aldehyde; alpha-n-Hexyl-beta-phenylacrolein. Jasmonal H . Hexyl cinnamic aldehyde	2569	129	101-86-0	216.32	C15 H20 O	Pale yellow liquid. jasmine like odour
687	p-Methoxycinnamaldehyde	p-Methoxycinnamaldehyde	p-Methoxycinnaldehyde	3567	11919	1963-36-6	162 18	C10 H10 O2	White to yellowish crystals, spicy floral odour
688	o-Methoxycinnamaldehyde	o-Methoxycinnamaldehyde	beta-(o-Methoxyphenyl) acrolein; 2'-Methoxycinnamaldehyde	3181	571	1504-74-1	162.19	C10 H10 O2	Pale yellow crystals, warm spicy floral odour
689	p-Methoxy-alpha-methyl-cinnamaldehyde	4'-Methoxy-2-methylcinnamaldehyde		3182	584	65405-67-6	176.21	C11 H12 O2	Deep yellow to orange liquid
690	Phenol	Phenol	Carbolic acid. Hydroxybenzene	3223	11811	108-95-2	94.11	C6 H6 O	White crystalline mass, sharp, medicinal, sweet, tarry odour
691	o-Cresol	o-Cresol	o-Cresylic acid; 1-Hydroxy-2-methylbenzene; o-Hydroxytoluene, o-Methylphenol	3480	618	95-48-7	108.14	C7 H8 O	Colourless to pale brown crystals

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
679	insoluble in water; soluble in oils	miscible	140 (20 mm Hg)	MS	95	5.0	1.526-1.532	1.003-1.009		55th/N	-
680	insoluble in water; soluble in oils	miscible	270	MS	90 (min 95% combined o- and p-isomers)	5.0	1.503-1.508	0.946-0.952		55th/N	-
681	slightly soluble in water	miscible	300	[req.]	97	1.0	1.504-1.511	0.954-0.963		55th/N,T	ID
682	insoluble in water; moderately soluble in oils	moderately soluble	154 (25 mm Hg)	IR	95	5.0	n/a	n/a	mp 41° (minimum)	55th/N	-
683	insoluble in water; soluble in oils	miscible	148 (27 mm Hg)	IR	95	5.0	1.598-1.607	1.034-1.040		55th/N	-
684	insoluble in water; soluble in oils	miscible	265	MS	98	5.0	1.539-1.547	0.977-0.984		55th/N	-
685	insoluble in water	miscible	284-287	IR	97	5.0	1.554-1.562	0.962-0.969		55th/N	-
686	insoluble in water; miscible in oils	miscible	174-175 (15 mm Hg)	IR	95	5.0	1.547-1.553	0.950-0.961		55th/N	-
687	insoluble in water; soluble in fats	moderately soluble	277	IR	96	4.0	n/a	n/a	mp: 57-58°	55th/N	-
688	slightly soluble in water	miscible	160-161 (12 mm Hg)	IR	94 (min. 95% combined aldehyde and corresponding acid)	5.0	n/a	n/a	mp. 45-46°; o-methoxycinnamic acid <3%	55th/N	-
689	insoluble in water; insoluble in oils	miscible	106-109 (0.1 mm Hg)	MS	95	5.0	1.625-1.632	0.989-0.996		55th/N	-
690	soluble in water	very soluble	182	IR	98	-	n/a	n/a	mp. 40-43°	55th/N	-
691	soluble in water	very soluble	191	IR	98	-	1.544-1.548	1.041-1.046	mp: 31-32° (liquid which may crystallize below 30°)	55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
692	m-Cresol	m-Cresol	m-Cresylic acid; 1-Hydroxy-3-methylbenzene; 3-Hydroxytoluene; m-Methylphenol	3530	617	108-39-4	108.14	C7 H8 O	Colourless to yellow-brown liquid, dry, tarry, medicinal-leathery, phenolic odour
693	p-Cresol	p-Cresol	p-Cresylic acid; 1-Hydroxy-4-methylbenzene; p-Hydroxytoluena; p-Methylphenol	2337	619	106-44-5	108.14	C7 H8 O	Colourless to pink crystals, tarry-smoky medicinal odour
694	p-Ethylphenol	4-Ethylphenol	4-Hydroxyethylbenzene	3156	550	123-07-9	122.17	C8 H10 O	Colourless needle like crystals, powerful, woody phenolic, medicinal, yet rather sweet odour
695	o-Propylphenol	2-Propylphenol	1-(2-Hydroxyphenyl)propane	3522	11908	644-35-9	136.19	C9 H12 O	Colourless oily liquid, phenolic odour
696	p-Propylphenol	4-Propylphenol	1-(4-Hydroxyphenyl)propane	3649		645-56-7	136.19	C9 H12 O	Colourless liquid, phenolic odour
697	2-Isopropylphenol	2-Isopropylphenol	o-Cumenol; 1-Hydroxy-2-isopropylbenzene; o-Isopropylphenol	3461	11234	88-69-7	136.19	C9 H12 O	Colourless liquid, phenolic odour
698	o-Tolyl acetate	o-Tolyl acetate	Acetyl o-cresol; o-Cresol acetate; o-Cresylic acetate	3072	2078	533-18-6	150.18	C9 H10 O2	Colourless liquid
699	p-Tolyl acetate	p-Tolyl acetate	Acetyl p-cresol; p-Cresyl acetate; p-Cresylic acetate	3073	226	140-39-6	150.18	C9 H10 O2	Clear, colourless liquid, strong floral odour
700	o-Tolyl isobutyrate	o-Tolyl isobutyrate	o-Cresyl isobutyrate; o-Tolyl 2-methylpropanoate	3753	681	36438-54-7	178.23	C11 H14 O2	Colourless liquid, floral phenolic odour
701	p-Tolyl isobutyrate	p-Tolyl isobutyrate	p-Cresyl isobutyrate; p-Methylphenyl isobutyrate; p-Tolyl 2-methylpropanoate	3075	304	103-93-5	178.23	C11 H14 O2	Colourless liquid, fruity odour
702	p-Tolyl 3-methylbutyrate	p-Tolyl isovalerate	p-Cresyl isovalerate; p-Cresyl 3-methylbutanoate; p-Tolyl isovalerate	3387	10545	55066-56-3	192.26	C12 H16 O2	Colourless liquid, tobacco-like, animal, sweet herbaceous odour
703	p-Tolyl octanoate	p-Tolyl octanoate	p-Cresyl octanoate; p-Cresyl caprylate; p-Tolyl caprylate	3733		59558-23-5	234.34	C15 H22 O2	Colourless oily liquid
704	p-Tolyl laurate	p-Tolyl laurate	p-Cresyl dodecanoate; p-Cresyl laurate; p-Tolyl dodecanoate	3076	378	10024-57-4	290.45	C19 H30 O2	Colourless oily liquid, mild, floral, sweet odour
705	p-Tolyl phenylacetate	p-Tolyl phenylacetate	p-Cresyl phenylacetate; p-Cresyl alpha-toluate; Narcissin; p-Tolyl alpha-toluate	3077	236	101-94-0	226.27	C15 H14 O2	White to off white crystals, faint lily, hyacinth, narcissus odour
706	2,5-Xylenol	2,5-Xylenol	1-Hydroxy-2,5-dimethylbenzene	3595	537	95-87-4	122.17	C8 H10 O	Colourless crystalline solid; Colourless needles
707	2,6-Xylenol	2,6-Xylenol	2-Hydroxy-1,3-dimethylbenzene	3249	11261	576-26-1	122.17	C8 H10 O	Colourless crystalline solid, sweet rooty odour
708	3,4-Xylenol	3,4-Xylenol	1-Hydroxy-3,4-dimethylbenzene	3596	11262	95-65-8	122.17	C8 H10 O	Colourless crystalline solid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
692	slightly soluble in water; soluble in oils	miscible	201	IR	98	-	1.537-1.543	1.028-1.033		55th/N	-
693	slightly soluble in water	very soluble	201-202	IR	99	-	n/a	n/a	mp: 32-36°	55th/N	-
694	slightly soluble in water; soluble in oils	very soluble	218-219	IR	99	-	n/a	n/a	mp: 47-48°	55th/N	-
695	slightly soluble in water, soluble in oils	miscible	224	IR	96	-	1.524-1.528	0.988-0.996		55th/N	-
696	insoluble in water; soluble in fat	miscible	232	IR	98	-	1.523-1.527	0.980-0.986		55th/N	-
697	slightly soluble in water	miscible	213-214	IR	98	-	1.525-1.530	0.989-0.999		55th/N	-
698	insoluble in water	miscible	208	[req.]	99	1.0	1.497-1.503	1.046-1.053		55th/N,T	ID
699	slightly soluble in water; soluble in oils	miscible	208-212	IR	98	1.0	1.499-1.503	1.044-1.052		55th/N	-
700	Insoluble in water; soluble in oils	miscible	107 (8 mm Hg)	IR	95	1.0	1.482-1.488	1.000-1.007		55th/N	-
701	insoluble in water; soluble in oils	miscible	237	IR	95	1.0	1.484-1.490	0.990-0.997		55th/N	-
702	insoluble in water, soluble in oils	miscible	103 (2 mm Hg)	IR	98	1.0	1.485-1489	0.977-0.987		55th/N	-
703	insoluble in water; soluble in oils	miscible	265	MS	96	1.0	1.478-1.488	0.952-0.960		55th/N	-
704	insoluble in water; soluble in oils	-	[req.]	[req.]	[req.]	-	[req.]	[req.]		55th/N,T	BP, ID, A, RI, SG
705	insoluble in water	moderately soluble	310	IR	97	1.0	n/a	n/a	mp: 71° (minimum)	55th/N	-
706	slightly soluble to soluble in water; soluble in fat	moderately soluble	211-212	IR	99	-	n/a	n/a	mp: 70° (minimum)	55th/N	-
707		very soluble	212	IR	99	-	n/a	n/a	mp: 45-49°	55th/N	-
708	slightly soluble in water; soluble in fat	moderately soluble	225	IR	98	-	n/a	n/a	mp: 62-68°	55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
709	Thymol	5-Methyl-2-(1-methylethyl)phenol	3-p-Cymenol; alpha-Cymophenol; 3-Hydroxy p-cymene; 1-Methyl-3-hydroxy-4- isopropylbenzene; 3-Methyl-6-isopropylphenol; Thyme camphor	3066	174	89-83-8	150.22	C10 H14 O	White crystals, powerful, sweet-medicinal, herbaceous, warm, aromatic odour
710	Carvacrol	2-Methyl-5-(1-methylethyl)phenol	p-Cymene-2-ol; Cymenphenol, 2-Hydroxy-p-cymene; Isopropyl-o-cresol; Isothymol; iso-Thymol	2245	2055	499-75-2	150.22	C10 H14 O	Colourless to pale yellow liquid, pungent, spicy odour
711	p-Vinylphenol	4-Ethenylphenol	p-Ethenylphenol; 4-Hydroxystyrene	3739	11257	2628-17-3	120.15	C8 H8 O	White solid, vanilla extract odour
712	Resorcinol	Resorcinol	m-Dihydroxybenzene	3589	11250	108-46-3	110.11	C6 H6 O2	White needle-like crystals
713	Guaiacol	o-Methoxyphenol	o-Hydroxyanisole; 1-Hydroxy-2-methoxybenzene; o-Methoxyphenol; o-Methylcatechol; 1-oxy-2-methoxybenzene; Pyrocatechol monomethyl ether; Pyroguaiac acid	2532	173	90-05-1	124.14	C7 H8 O2	Colourless to amber crystals, powerful, smoke-like, somewhat medicinal odour
714	o-(Ethoxymethyl)phenol	o-(Ethoxymethyl)phenol	2-(Ethoxymethyl)hydroxybenzene; o-Hydroxybenzyl ethyl ether; alpha-Ethoxy-o-cresol	3485	11905	20920-83-6	152.19	C9 H12 O2	Colourless to yellowish oily liquid, sweet smokey, vanillic odour
715	2-Methoxy-4-methylphenol	2-Methoxy-p-cresol	Creosol; Homocatechol monoethyl ether; 1-Hydroxy-2-methoxy-4-methylbenzene; 2-Methoxy-p-cresol; 4-Methylguaiacol; Valspice	2671	175	93-51-6	138.17	C8 H10 O2	Colourless to yellowish liquid, sweet, spicy, slightly vanilla-like odour
716	4-Ethylguaiacol	4-Ethylguaiacol	Homocreosol, 1-Hydroxy-2-methoxy-4-ethylbenzene	2436	176	2785-89-9	152.19	C9 H12 O2	Colourless, oily liquid, warm, sweet, spicy, medicinal odour
717	2-Methoxy-4-propylphenol	2-Methoxy-4-propylphenol	4-Propylguaiacol; 5-Propyl-o-hydroxyanisole; 4-Propyl-o-methoxyphenol; Dihydroeugenol	3598		2785-87-7	166.22	C10 H14 O2	Colourless oily liquid, warm, spicy, sweet, and slightly floral balsamic odour
718	Guaiacyl acetate	2-Methoxyphenol acetate	1-Acetoxy-2-methoxybenzene; Acetyl guaiacol; o-Methoxyphenyl acetate; o-Acetoxyanisole	3687	552	613-70-7	166.18	C9 H10 O3	Colourless to pale straw coloured liquid, woody, dry, slightly green odour
719	Guaiacyl phenylacetate	2-Methoxyphenyl phenylacetate	Guaiacol phenylacetate; o-Methylcatechol phenylacetate; o-Methoxyphenol phenylacetate	2535	238	4112-89-4	242.27	C15 H14 O3	Amber viscous liquid. When pure it forms colourless crystals with heavy, rather dry, woody, herbaceous odour
720	Hydroquinone monoethyl ether	p-Ethoxyphenol	1-Ethoxy-4-hydroxybenzene; p-Ethoxyphenol; p-Hydroxyphenetole	3695	2258	622-62-8	138.17	C8 H10 O2	White or colourless crystals, sweet herbaceous odour reminiscent of anise and fennel
721	2,6-Dimethoxyphenol	2,6-Dimethoxyphenol	2-Hydroxy-1,3-dimethoxybenzene; Pyrogallol 1,3-dimethyl ether; Syringol	3137	2233	91-10-1	154.17	C8 H10 O3	White or colourless crystals, woody medicinal rather dry odour
722	4-Methyl-2,6-dimethoxyphenol	2,6-Dimethoxy-p-cresol	2,6-Dimethoxy-p-cresol, 4-Methylsyringol	3704		6638-05-7	168.19	C9 H12 O3	Pale yellow semi-solid, phenolic medicinal odour

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
709	slightly soluble in water; soluble in oils	moderately soluble	232-233	IR	98	-	n/a	n/a	mp: 48° (minimum)	55th/N	-
710	insoluble in water; miscible in oils	miscible	236-238	IR	98	-	1.521-1.528	0.974-0.979		55th/N	-
711	soluble in water; slightly soluble in fat	moderately soluble	[req.]	MS	99	-	n/a	n/a	mp: 68°	55th/N,T	BP
712	soluble in water	moderately soluble	277-281	IR	98	-	n/a	n/a	mp: 109°	55th/N	-
713	slightly soluble in water	very soluble	203-206	IR	99	-	1.540-1.545	1.129-1.140	mp: 28° (liquid which may crystallize)	55th/N	-
714	slightly soluble in water; soluble in oils	miscible	111-113 (20 mm Hg)	MS	99	-	1.517-1.523	1.047-1.052		55th/N	-
715	slightly soluble in water	miscible	220-222	IR	98	-	1.534-1.538	1.089-1.096		55th/N	-
716	slightly soluble in water; miscible in oils	miscible	229-235	IR	98	-	1.524-1.534	1.056-1.066		55th/N	-
717	slightly soluble in water; soluble in fat	miscible	250	IR	98	-	1.520-1.525	1.034-1.040		55th/N	-
718	insoluble to slightly soluble in water	miscible	240-241	IR	98	1.0	1.507-1.513	1.127-1.134		55th/N	-
719	insoluble in water	very soluble	[req.]	IR	97	1.0	n/a	n/a	mp: 38° (minimum)	55th/N,T	BP
720	slightly soluble to soluble in water; soluble in oils	moderately soluble	246-247	[req.]	95	-	n/a	n/a	mp: 64° (minimum)	55th/N,T	ID
721	slightly soluble in water; soluble in oils	moderately soluble	261-262	IR	98	-	n/a	n/a	mp: 53° (minimum)	55th/N	-
722	insoluble in water; soluble in fat	moderately soluble	145-146 (12 mm Hg)	IR	97	-	n/a	n/a	mp: 37-42°	55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
723	4-Ethyl-2,6-dimethoxyphenol	4-Ethyl-2,6-dimethoxyphenol	2,6-Dimethoxy-4-ethylphenol; 4-Ethylsyringol	3671	11231	14059-92-8	182.22	C10 H14 O3	Water white liquid
724	4-Propyl-2,6-dimethoxyphenol	4-Propyl-2,6-dimethoxyphenol	4-Propylsyringol	3729		6766-82-1	196.25	C11 H16 O3	Water white liquid
725	2-Methoxy-4-vinylphenol	2-Methoxy-4-vinylphenol	4-Hydroxy-3-methoxystyrene; p-Vinylcatechol-o-methyl ether; p-Vinylguaiacol	2675	177	7786-61-0	150.18	C9 H10 O2	Colourless or pale straw oily liquid, powerful, spicy, clove-like roasted peanut odour
726	4-Allyl-2,6-dimethoxyphenol	4-Allyl-2,6-dimethoxyphenol	4-Allylsyringol; 2,6-Dimethoxy-4-(2-propenyl) phenol; 6-Methoxy eugenol	3655	11214	6627-88-9	194.23	C11 H14 O3	Clear pale yellow liquid, roasted meaty bacon odour
727	2-Hydroxyacetophenone	2'-Hydroxyacetophenone	o-Acetylphenol; o-Hydroxyacetophenone	3548	11784	118-93-4	136.15	C8 H8 O2	Colourless liquid
728	4-(p-Hydroxyphenyl)-2-butanone	4-(4-Hydroxyphenyl)butan-2-one	p-Hydroxybenzylacetone; 1-p-Hydroxyphenyl-3-butanone; Raspberry ketone; Rastone; Oxyphenylon; Oxanone	2588	755	5471-51-2	164.20	C10 H12 O2	White needle like crystals or granule crystalline material with sweet fruity, warm odour resembling raspberry preserve
729	Dihydroxyacetophenone	1-Phenylethanone, dihydroxy derivative	1-(x,y-Dihydroxyphenyl) ethanone, Dioxyacetophenone, Dihydroxyphenyl methyl ketone	3662	11884	28631-86-9	152.15	C8 H8 O3	Yellow needles or crystals
730	Zingerone	4-(4-Hydroxy-3-methoxyphenyl)-2-butanone	4-Hydroxy-3-methoxybenzylacetone, 2-(4-Hydroxy-3-methoxyphenyl)ethyl methyl ketone, Vanillylacetone	3124	139	122-48-5	194.23	C11 H14 O3	Yellowish to yellow-brown crystalline mass, sweet, spicy, warm, heavy floral, mildly animal balsamic, vanilla like odour
731	4-(p-Acetoxyphenyl)-2-butanone	4-(p-Hydroxyphenyl)-2-butanone acetate	4-(3-Oxobutyl)phenylacetate; p-(2-Acetylethyl) phenylacetate	3652		3572-06-3	206.24	C12 H14 O3	Yellow liquid, sweet raspberry fruity odour
732	Vanillylidene acetone	Methyl 3-methoxy-4-hydroxystyrl ketone		3738	691	1080-12-2	192.21	C11 H12 O3	Yellowish, needle like crystals, sweet warm and tenacious odour
733	4-(1,1-Dimethylethyl) phenol	p-tert-Butylphenol	4-tert-Butylphenol; p-tert-Butylphenol, 1-Hydroxy-4-tert-butylbenzene			98-54-4	150.22	C10 H14 O	White needle-like crystals, phenolic odour
734	Phenyl acetate	Phenyl acetate	Phenol acetate, Acetoxybenzene		10878	122-79-2	136.15	C8 H8 O2	Colourless liquid
735	2-Phenylphenol	Biphenyl-2-ol	Anthrapole 73; Dowicide 1; o-Hydroxy biphenyl; Torsite; Xenol; o-Phenylphenol; OPP, 2-Biphenylol			90-43-7	170.21	C12 H10 O	White to light purple crystals
736	Phenyl salicylate	2-Hydroxybenzoic acid, phenyl ester	Salol		11814	118-55-8	214.22	C13 H10 O3	White crystalline solid
737	2,3,6-Trimethylphenol	2,3,6-Trimethylphenol	Methyl xylenol-2,3,6; 3-Hydroxypseudocumene			2416-94-6	136.19	C9 H12 O	White crystalline solid

No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
723	insoluble in water, soluble in fat	miscible	106 (0.2 mm Hg)	MS	98	-	1.536-1.537	[req.]		55th/N,T	SG
724	insoluble in water; soluble in fat	miscible	115 (0.38 mm Hg)	IR (on paper)	98	-	1.529-1.530	[req.]		55th/N,T	SG
725	insoluble in water; soluble in oils	miscible	224	IR	96	-	1.534-1.538	1.090-1.096		55th/N	-
726	insoluble in water; soluble in fat	miscible	168 (11 mm Hg)	IR (on paper)	98	-	1.548-1.550	[req.]		55th/N,T	SG
727	slightly soluble in water; soluble in fat	miscible	215-220	IR	95	-	1.556-1.560	1.127-1.133		55th/N	-
728	insoluble in water, soluble in oils	moderately soluble	decomposes	IR	96	-	n/a	n/a	mp: 80° (minimum)	55th/N	-
729	(3,4-isomer) insoluble to slightly soluble in water; (2,5-isomer) slightly soluble in water; (3,5-isomer) soluble in water	moderately soluble	decomposes	[req.]	[req.]	-	n/a	n/a	mp: 90° (minimum)	55th/N,T	ID, A
730	slightly soluble in water	moderately soluble	187-188 (14 mm Hg)	IR	95	-	n/a	n/a	mp: 40-41°	55th/N	-
731	insoluble in water; soluble in fat	miscible	155 (2.5 mm Hg)	IR	93 (min. 95% combined o- and p-isomers)	-	1.506-1.512	1.096-1.100	contains 2-5% ortho isomer	55th/N	-
732	slightly soluble in water	moderately soluble	decomposes	[req.]	97	-	n/a	n/a	mp: 129-130°	55th/N,T	ID
733	insoluble in water; soluble in ethanol; soluble in ether	moderately soluble	236	IR (on paper)	98	-	n/a	n/a	mp: 98-101°	55th/N	-
734	insoluble in water; miscible in alcohol	miscible	195-196	IR	97	1.0	1.500-1.506	1.073-1.079		55th/N	-
735	insoluble in water	moderately soluble	282	[req.]	99	-	n/a	n/a	mp: 57-58°	55th/N,T	ID
736	insoluble in water; soluble in 50% Heptane	moderately soluble	172-173 (12 mm Hg)	IR	99	1.0	n/a	n/a	mp: 41-43°	55th/N	-
737	insoluble in water	50% soluble in ethyl alcohol	[req.]	IR (on paper)	99	-	n/a	n/a	mp: 63-64°	55th/N,T	BP

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
739	Furfuryl acetate	2-Furanmethanol acetate	2-Furyl carbinyl acetate	2490	2065	623-17-6	140.14	$C_7H_8O_3$	Colourless oily liquid, mild, ethereal-floral fruity odour
740	Furfuryl propionate	2-Furanmethanol propionate	Furfuryl propanoate	3346	10646	623-19-8	154.17	$C_8H_{10}O_3$	Oily liquid which darkens on exposure to light, green banana odour
741	Furfuryl pentanoate	Pentanoic acid, 2-furanylmethyl ester	alpha-Furfuryl pentanoate; alpha-Furfuryl valerate	3397	10647	36701-01-6	182.22	$C_{10}H_{14}O_3$	Colourless oily liquid, sweet overripe fruit odour
742	Furfuryl octanoate	Octanoic acid, 2-furanylmethyl ester	alpha-Furfuryl caprylate, alpha-Furfuryl octanoate	3396	10645	39252-03-4	224.30	$C_{13}H_{20}O_3$	
743	Furfuryl 3-methylbutanoate	3-Methylbutanoic acid, 2-furanylmethyl ester	Furfuryl isovalerate	3283	10642	13678-60-9	182.22	$C_{10}H_{14}O_3$	
745	5-Methylfurfural	5-Methyl-2-furfuraldehyde		2702	119	620-02-0	110.11	$C_6H_6O_2$	Colourless liquid, spicy-sweet, warm and slightly caramellic odour
746	Methyl 2-furoate	2-Furoic acid, methyl ester	Methyl furoate; Methyl pyromucate	2703	358	611-13-2	126.11	$C_6H_6O_3$	Colourless to pale yellow liquid, berry, fruity, winey, heavy odour
747	Propyl 2-furoate	2-Furoic acid, propyl ester	Propyl furan-2-carboxylate, n-Propyl pyromucate	2946	359	615-10-1	154.17	$C_8H_{10}O_3$	Colourless liquid, sweet-oily, herbaceous-earthy odour
748	Amyl 2-furoate	2-Furoic acid, pentyl ester	Amyl furan-2-carboxylate; Pentyl furan-2-carboxylate	2072	2109	1334-82-3	182.22	$C_{10}H_{14}O_3$	Colourless to pale yellow liquid, sweet, caramellic, winey, somewhat herbaceous odour
749	Hexyl 2-furoate	2-Furoic acid, hexyl ester	Hexyl furan-2-carboxylate	2571	361	39251-86-0	196.25	$C_{11}H_{16}O_3$	Colourless to pale straw coloured liquid, fruity-earthy, yet sweet pear-like odour
750	Octyl 2-furoate	2-Furoic acid, octyl ester	Octyl 2-furancarboxylate	3518	10864	39251-88-2	224.30	$C_{13}H_{20}O_3$	Colourless to pale straw liquid, sweet fruity heavy odour
751	2-Benzofurancarboxaldehyde	2-Benzofurancarboxaldehyde	2-Formylbenzofuran	3128	2247	4265-16-1	146.15	$C_9H_6O_2$	Crystalline solid, bitter almond odour
752	2-Phenyl-3-carbethoxyfuran	Ethyl 2-phenyl-3-furoate	Phenyl oxaromate	3468	2309	50626-02-3	216.24	$C_{13}H_{12}O_3$	
753	Pulegone	p-Menth-4(8)-en-3-one	delta-4(8)-p-Menthen-3-one, 1-Isopropylidene-4-methyl-2-cyclohexanone, 1-Methyl-4-isopropylidene-3-cyclohexanone; 5-Methyl-2-(1-methylethylidene)cyclohexanone	2963	2050	89-82-7	152.24	$C_{10}H_{16}O$	Colourless to yellow liquid, herbaceous-minty, resinous odour
754	Isopulegone	p-Menth-8-en-3-one, trans-	lambda-8(9)-p-Menthen-3-one; 1-Isopropenyl-4-methyl-2-cyclohexanone; 1-Methyl-4-isopropenyl-3-cyclohexanone	2964	2051	29606-79-9	152.24	$C_{10}H_{16}O$	Colourless to yellow liquid, minty-woody, mildly green odour

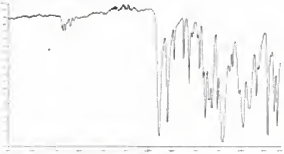
No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive Index	Specific gravity	Other Requirements	JECFA	Data required
739	insoluble in water; soluble in oils	miscible	175-177	IR	97	1.0	1.457-1.466	1.110-1.119		55th/N	-
740	slightly soluble in water	miscible	195-196	[req.]	98	1.0	1.457-1.464	1.076-1.086		55th/N,T	ID
741	Insoluble in water	miscible	228-229	IR	98 by ester determination	1.0	1.457-1.462	1.024-1.031		55th/N,T	A(e)
742	insoluble in water; soluble in oils	miscible	139 (10 mm Hg)	IR	98 by ester determination	1.0	1.456-1.464	0.980-0.989		55th/N,T	A(e)
743	insoluble in water soluble in oils	miscible	97-98 (11 mm Hg)	IR	98 by ester determination	1.0	1.456-1.464	1.014-1.023		55th/N,T	A(e)
745	slightly soluble in water; soluble in oils	miscible	187	IR	97	1.0	1.525-1.532	1.098-1.108		55th/N	-
746	insoluble to slightly soluble in water; soluble in oils	miscible	181	IR	98	1.0	1.485-1.490	1.176-1.181		55th/N	-
747	slightly soluble in water; soluble in oils	miscible	211	MS	97	1.0	1.471-1.475	1.067-1.075		55th/N	-
748	insoluble in water	miscible	95-97 (1 mm Hg)	[req.]	98	1.0	1.469-1.475	1.031-1.038		55th/N,T	ID
749	insoluble in water; soluble in oils	miscible	252	[req.]	97	1.0	1.468-1.473	1.015-1.020		55th/N,T	ID
750	insoluble in water; miscible in fat	miscible	126-127 (1 mm Hg)	[req.]	98	1.0	1.466-1.472	0.984-0.990		55th/N,T	ID
751	insoluble in water	slightly soluble	130-131 (13 mm Hg)	MS	96	3.0	n/a	n/a		55th/N	-
752	insoluble in water; soluble in oils	-	148-154 (6 mm Hg)	[req.]	99	1.0	[req.]	[req.]		55th/N,T	ID, RI, SG
753	insoluble in water, soluble in oils; miscible to soluble in alcohol	miscible	224	IR	95	1.0	1.483-1.491	0.927-0.939		55th/N	-
754	insoluble in water; soluble in alcohol and oils	miscible	208	MS	95	-	1.465-1.473	0.925-0.932		55th/N	-

No	Name	Chemical name (Systematic name)	Synonyms	FEMA	COE	CAS	Mol Wt	Formula	Physical form/odour
755	Isopulegol	p-Menth-8-en-3-ol	8(9)-p-Menthen-3-ol; 1-Methyl-4-isopropenylcyclohexan-3-ol	2962	2033	89-79-2	154.25	C10 H18 O	Colourless liquid, minty-herbaceous, bitter-sweet, harsh, camphoraceous odour
756	Isopulegyl acetate	Isopulegyl acetate	"Acetylated citronellal"; 1-Methyl-4-isopropenylcyclohexan-3-yl acetate	2965	2067	57576-09-7	196.29	C12 H20 O2	Colourless liquid, fresh, green-minty, leafy, sweet fruity odour
757	p-Menth-1,4(8)-dien-3-one	3-Methyl-6-(1-methylethylidene)cyclohex-2-en-1-one	Piperitenone; 1-Methyl-4-isopropylidene-1-cyclohexen-3-one	3560	11189	491-09-8	150.22	C10 H14 O	Yellow to amber oily liquid, powerful sharp, minty, phenolic odour
758	Menthofuran	4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran		3235	2265	494-90-6	150.22	C10 H14 O	Bluish liquid, odour similar to that of menthol
759	Furfuryl butyrate	Butanoic acid, 2-furanylmethyl ester	2-Furylmethyl butanoate		638	623-21-2	168.19	C9 H12 O3	Oily liquid, green butyric rancid odour
760	Cinnamyl benzoate	Cinnamyl benzoate			743	5320-75-2	238.29	C16 H14 O2	White crystalline powder, balsamic, aromatic, spicy odour

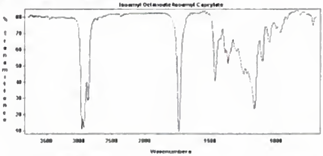
No	Solubility	Solubility in ethanol	Boiling point (°C)	ID Test	Assay min %	Acid value max	Refractive index	Specific gravity	Other Requirements	JECFA	Data required
755	slightly soluble in water; soluble in oils	miscible	218	IR	95 (total of isomers <1% citronellal)	1.0	1.468-1.477	0.904-0.913		55th/N	-
756	insoluble in water; soluble in oils	miscible	232; 104-105 (10 mm Hg)	IR	95 (total of isomers)	1.0	1.454-1.457	0.929-0.936		55th/N	-
757	insoluble in water; soluble in oils	miscible	233	MS	95 (total of isomers)	-	1.472-1.478	0.976-0.983		55th/N	-
758	insoluble in water; soluble in oils	miscible	196; 95 (20 mm Hg); 80 (18 mm Hg) 90-92 (3 mm Hg)	IR	99	-	1.481-1.486	0.960-0.970		55th/N	-
759	insoluble in water	miscible	212	[req.]	99	1.0	[req.]	[req.]		55th/N,T	ID, RI, SG
760	insoluble in water; soluble in oils	miscible	335	[req.]	98	1.0	n/a	n/a	mp: 31°	55th/N,T	ID

Infrared (IR) and other spectra of certain flavouring agents

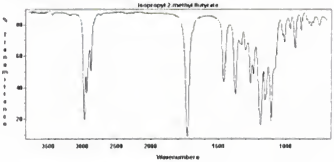
19 Allyl cinnamate



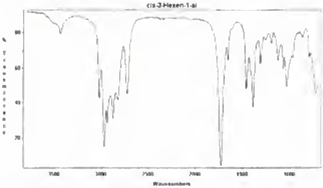
47 Isoamyl octanoate



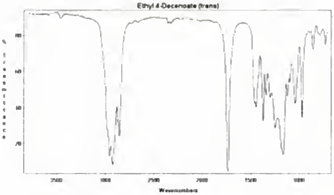
210 Isopropyl 2-methylbutyrate



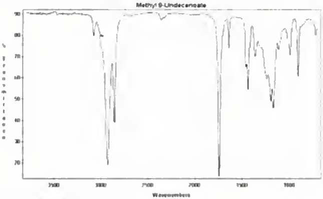
316 cis-3-Hexenal



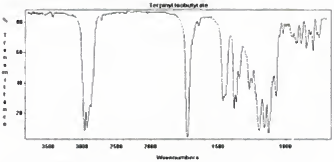
341 Ethyl trans-4-decenoate



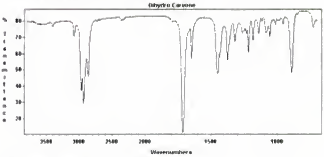
342 Methyl 9-undecenoate



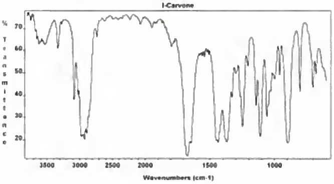
371 Terpinyl butyrate



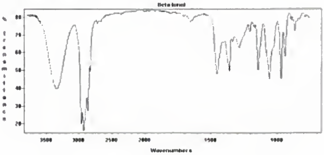
377 Dihydrocarvone



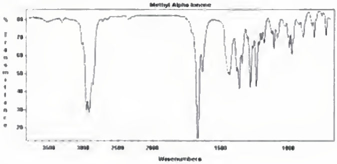
380.1 l-Carvone



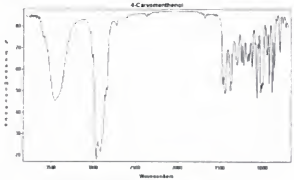
392 beta-Ionol



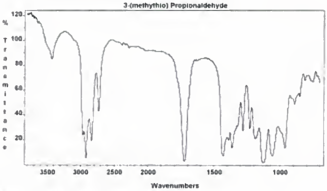
398 Methyl-alpha-ionone



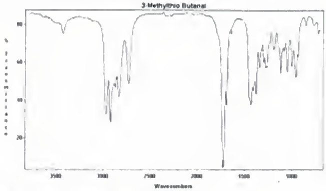
439 4-Carvomenthenol



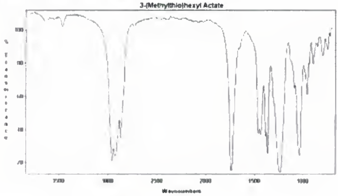
466 3-(Methylthio)propionaldehyde



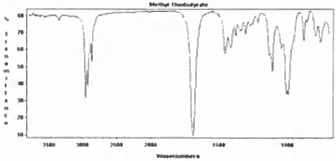
467 3-(Methylthio)butanal



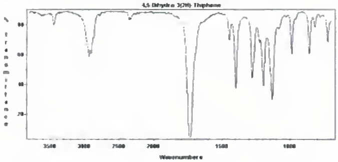
481 3-(Methylthio)hexyl acetate



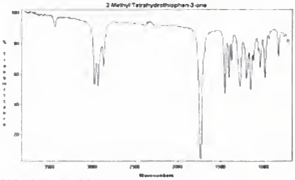
484 Methyl thiobutyrate



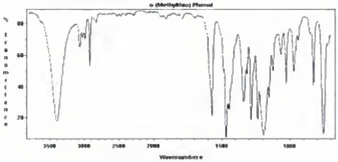
498 4,5-Dihydro-3(2H) thiophenone



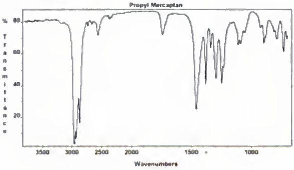
499 2-Methyltetrahydrothiophen-3-one



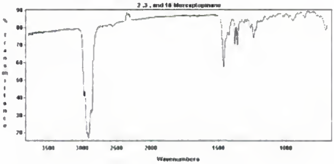
503 o-(Methylthio)phenol



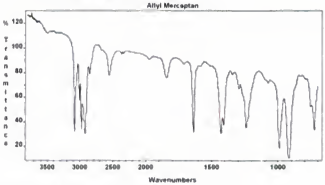
509 Propanethiol



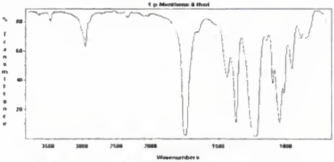
520 2,3,or 10-Mercaptopinane



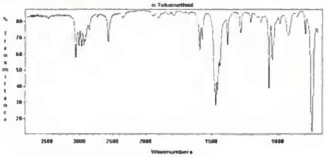
521 Allyl mercaptan



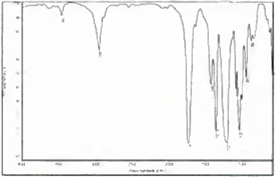
523 1-p-Menthene-8-thiol



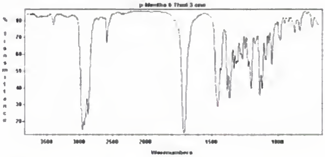
528 o-Toluenethiol



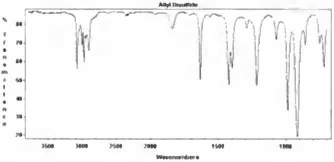
558 3-Mercapto-2-butanone



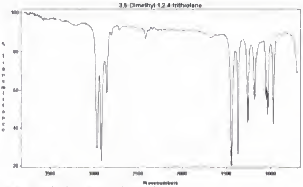
561 p-Mentha-8-thiol-3-one



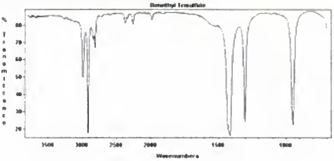
572 Allyl disulfide



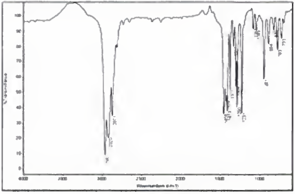
573 3,5-Dimethyl-1,2,4-trithiolane



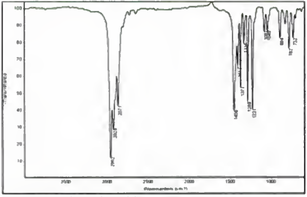
582 Dimethyl trisulfide



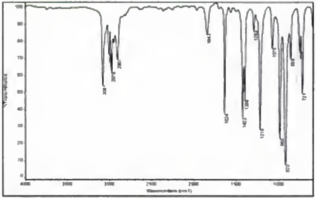
584 Methyl propyl trisulfide



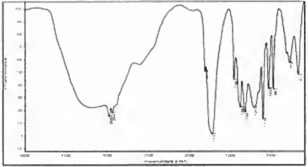
585 Dipropyl trisulfide



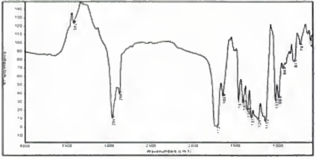
587 Diallyl trisulfide



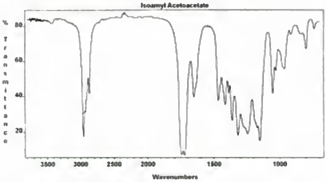
589 2-Oxobutyric acid



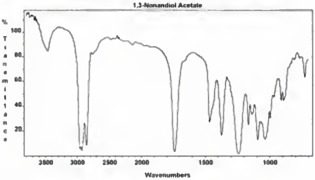
597 Isobutyl acetoacetate



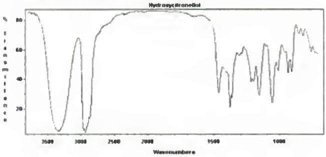
598 Isoamyl acetoacetate



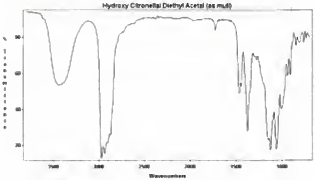
605 1,3-Nonanediol acetate (mixed esters)



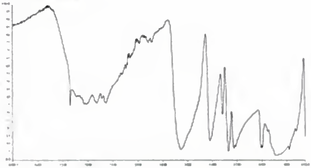
610 Hydroxycitronellol



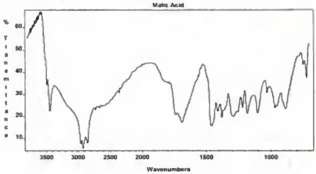
613 Hydroxycitronellal diethyl acetal



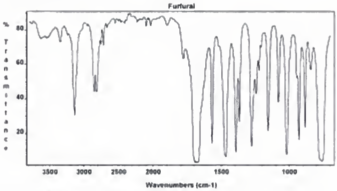
618 Fumaric acid



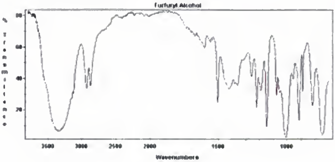
619 l-Malic acid



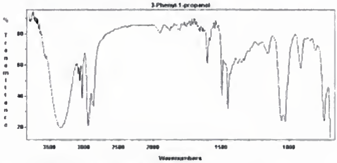
450 Furfural



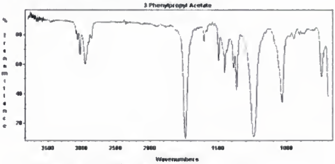
451 Furfuryl alcohol



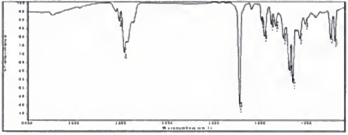
636 3-Phenyl-1-propanol



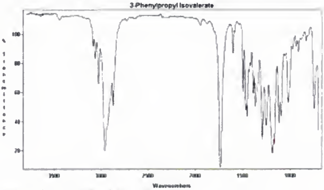
638 3-Phenylpropyl acetate



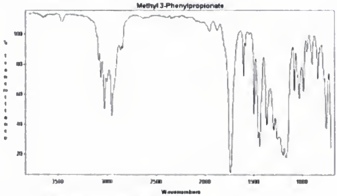
640 3-Phenylpropyl isobutyrate



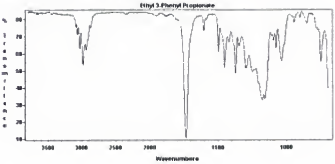
641 3-Phenylpropyl isovalerate



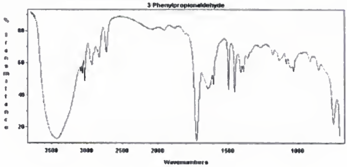
643 Methyl 3-phenylpropionate



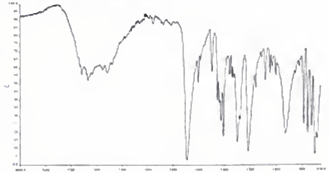
644 Ethyl 3-phenylpropionate



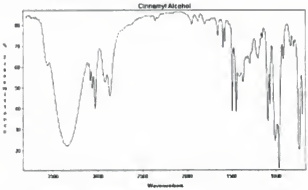
645 3-Phenylpropionaldehyde



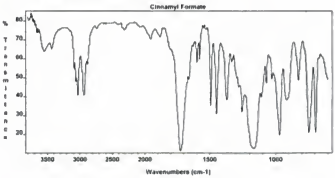
646 3-Phenylpropionic acid



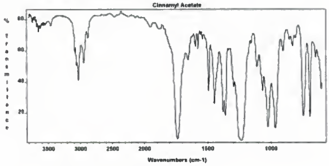
647 Cinnamyl alcohol



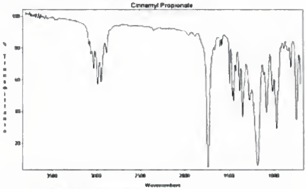
649 Cinnamyl formate



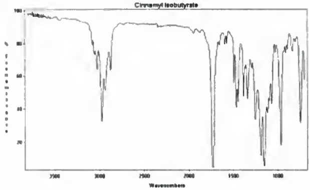
650 Cinnamyl acetate



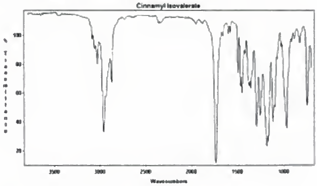
651 Cinnamyl propionate



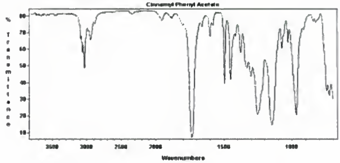
653 Cinnamyl isobutyrate



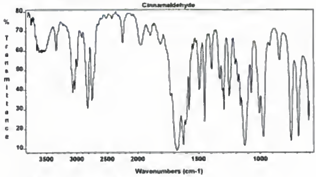
654 Cinnamyl isovalerate



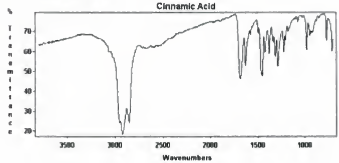
655 Cinnamyl phenylacetate



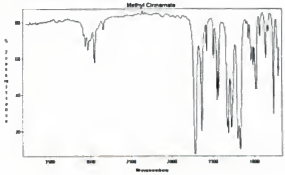
656 Cinnamaldehyde



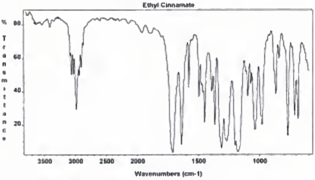
657 Cinnamic acid



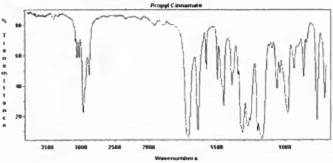
658 Methyl cinnamate



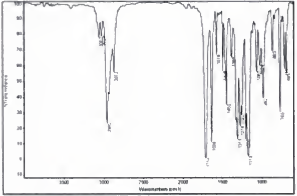
659 Ethyl cinnamate



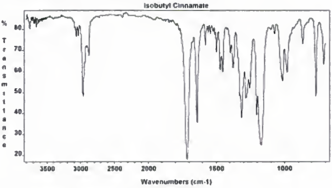
660 Propyl cinnamate



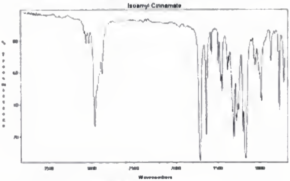
663 Butyl cinnamate



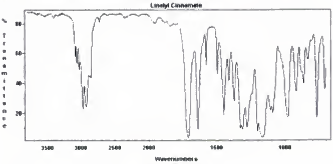
664 Isobutyl cinnamate



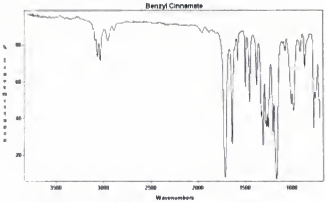
665 Isoamyl cinnamate



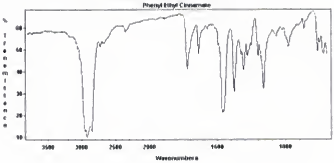
668 Linalyl cinnamate



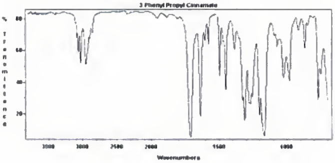
670 Benzyl cinnamate



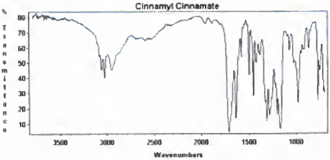
671 Phenethyl cinnamate



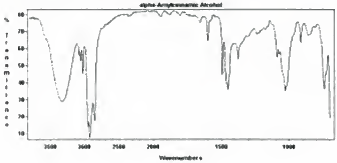
672 3-Phenylpropyl cinnamate



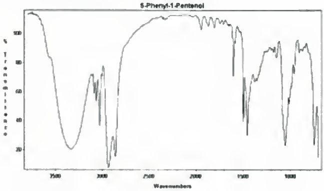
673 Cinnamyl cinnamate



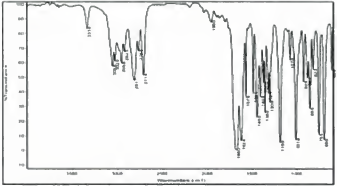
674 alpha-Amylcinnamyl alcohol



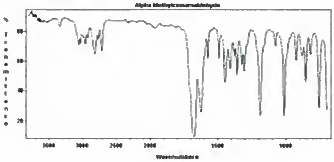
675 5-Phenylpentanol



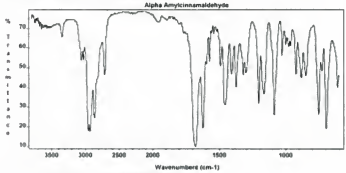
682 p-Methylcinnamaldehyde



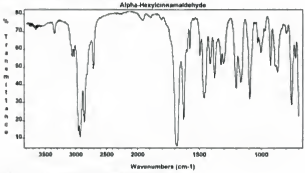
683 alpha-Methylcinnamaldehyde



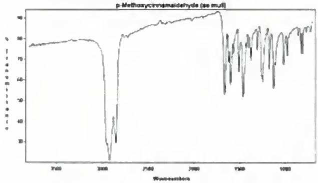
685 alpha-Amylcinnamaldehyde



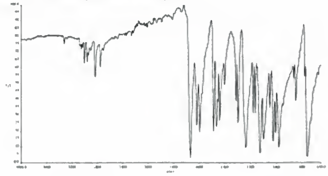
686 alpha-Hexylcinnamaldehyde



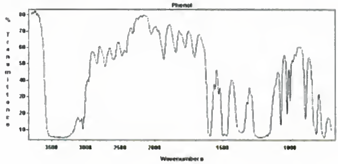
687 p-Methoxycinnamaldehyde



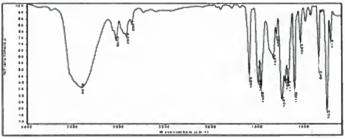
688 o-Methoxycinnamaldehyde



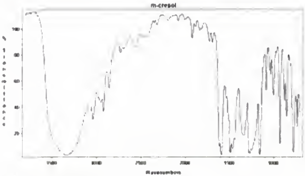
690 Phenol



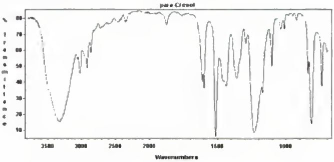
691 o-Cresol



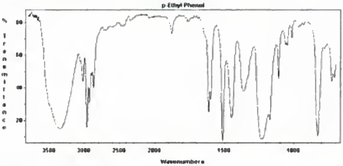
692 m-Cresol



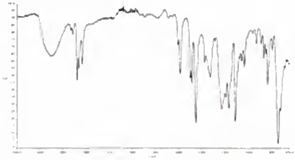
693 p-Cresol



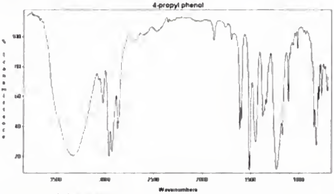
694 p-Ethylphenol



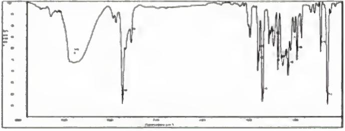
695 o-Propylphenol



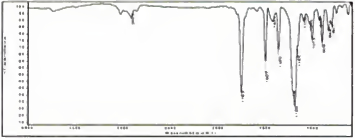
696 p-Propylphenol



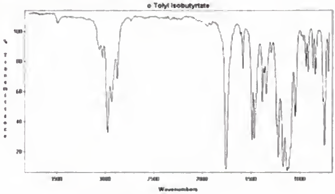
697 2-Isopropylphenol



699 p-Tolyl acetate



700 o-Tolyl isobutyrate



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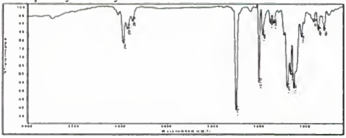
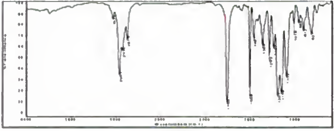
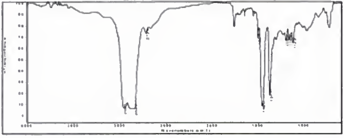


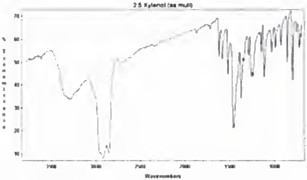
702 p-Tolyl 3-methylbutyrate



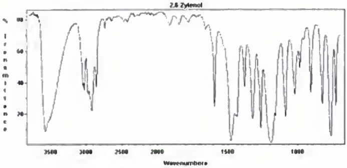
705 p-Tolyl phenylacetate



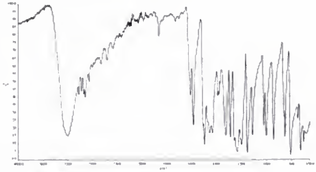
706 2,5-Xylenol



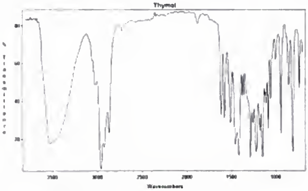
707 2,6-Xylenol



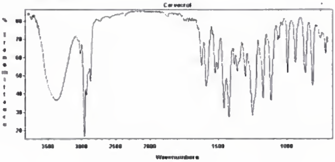
708 3,4-Xylenol



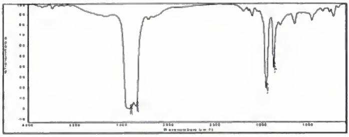
709 Thymol



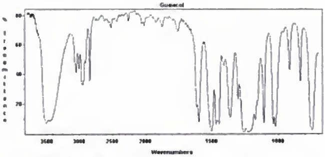
710 Carvacrol



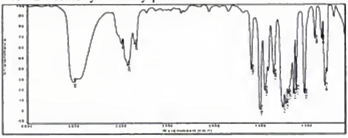
712 Resorcitol



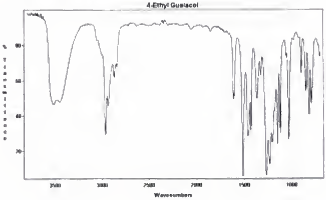
713 Guaiacol



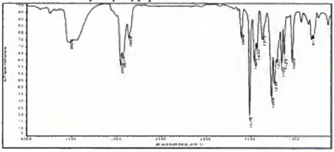
715 2-Methoxy-4-methylphenol



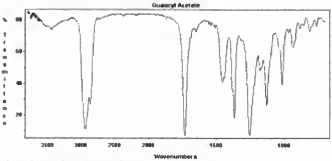
716 4-Ethylguaiacol



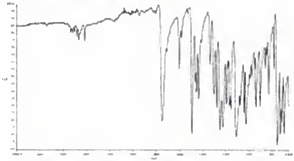
717 2-Methoxy-4-propylphenol



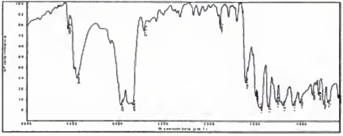
718 Guaiacyl acetate



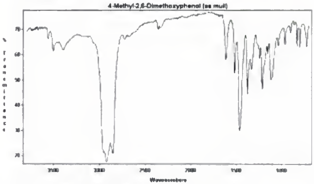
719 Guaiacyl phenylacetate



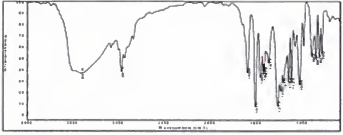
721 2,6-Dimethoxyphenol



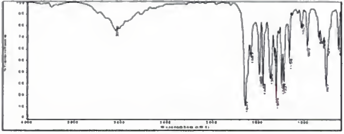
722 4-Methyl-2,6-dimethoxyphenol



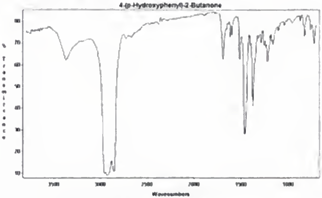
725 2-Methoxy-4-vinylphenol



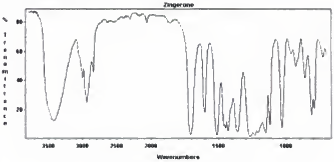
727 2-Hydroxyacetophenone



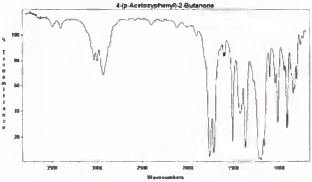
728 4-(p-Hydroxyphenyl)-2-butanone



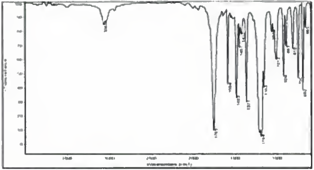
730 Zingerone



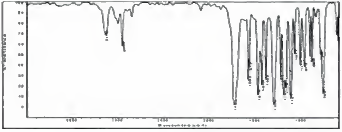
731 4-(p-Acetoxyphenyl)-2-butanone



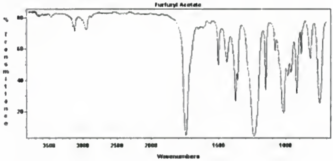
734 Phenyl acetate



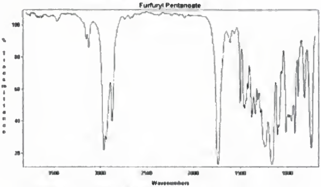
746 Methyl 2-furoate



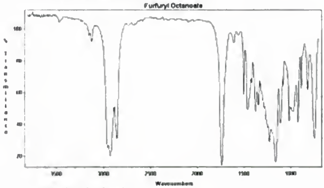
739 Furfuryl acetate



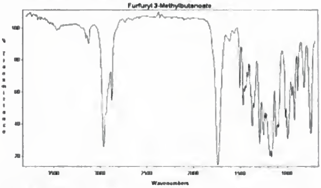
741 Furfuryl pentanoate



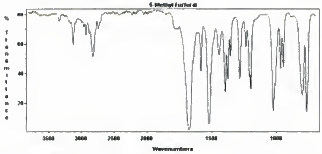
742 Furfuryl octanoate



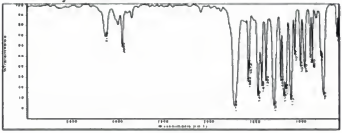
743 Furfuryl 3-methylbutanoate



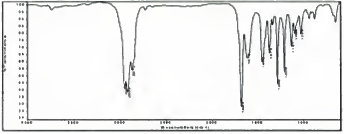
745 5-Methylfurfural



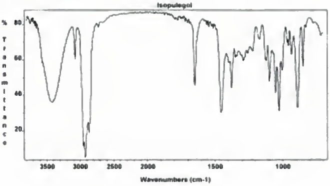
746 Methyl 2-furoate



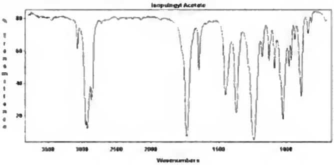
753 Pulegone



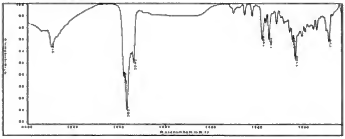
755 Isopulegol



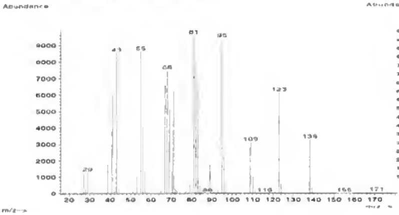
756 Isopulegyl acetate



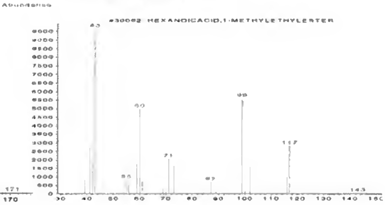
758 Menthofuran



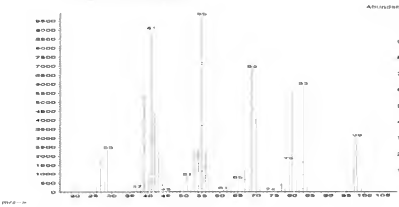
74 Rhodinyl isobutyrate



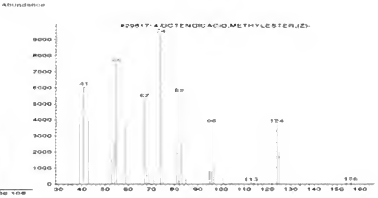
308 Isopropyl hexanoate



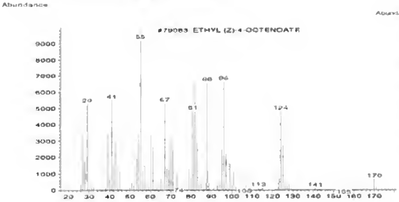
319 cis-4-Hexenal



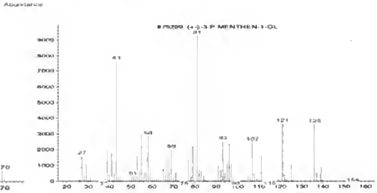
337 Methyl cis-4-octenoate



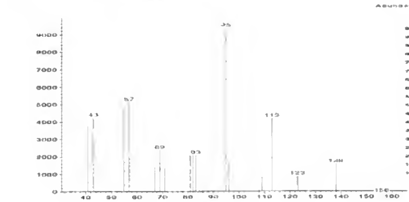
338 Ethyl cis-4-octenoate



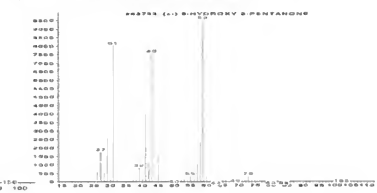
373 p-Menth-3-en-1-ol



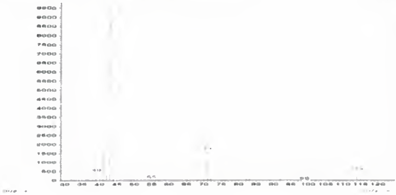
376 p-Menthan-2-ol



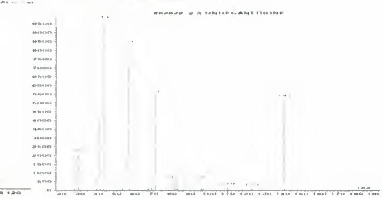
409 3-Hydroxy-2-pentanone



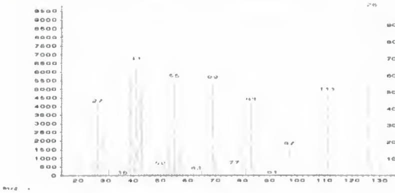
411 4-Methyl-2,3-pentanedione



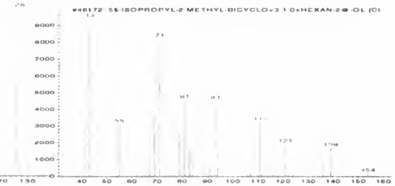
417 2,3-Undecadione



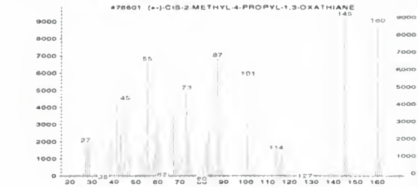
421 3,5-Dimethyl-1,2-cyclo-pentanedione



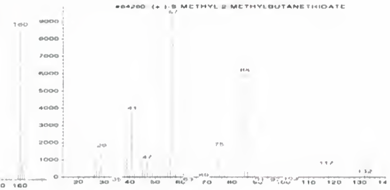
441 4-Thyjanol



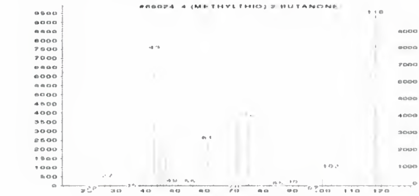
464 2-Methyl-4-propyl-1,3-oxathiane



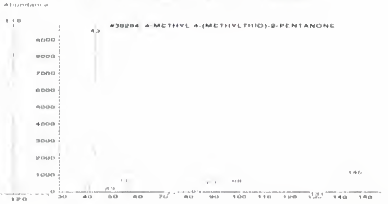
486 S-Methyl 2-methylbutanethioate



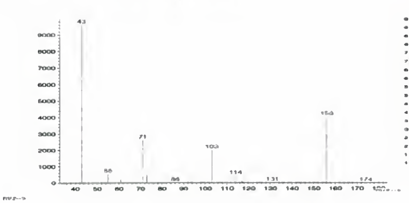
497 4-(Methylthio)-2-butanone



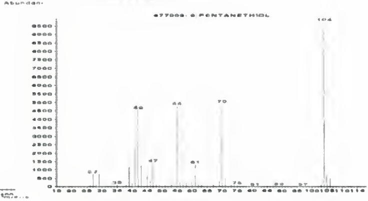
500 4-(Methylthio)-4-methyl-2-pentanone



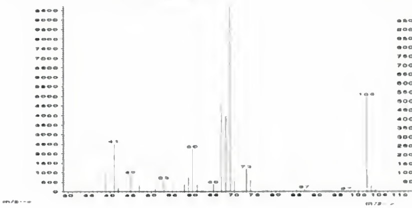
502 Di(butan-3-one-1-yl)sulfide



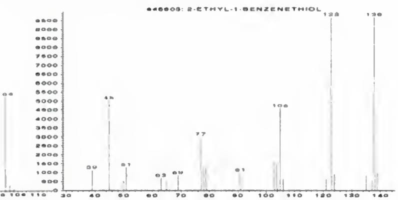
514 2-Pentanethiol



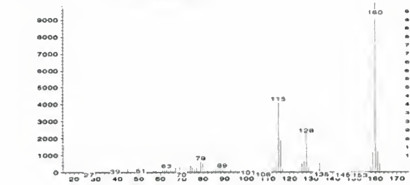
516 Cyclopentanethiol



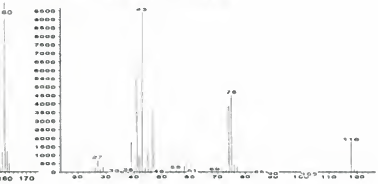
529 2-Ethylthiophenol



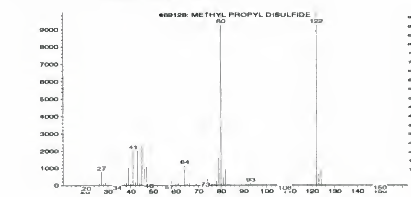
531 2-Naphthalenethiol



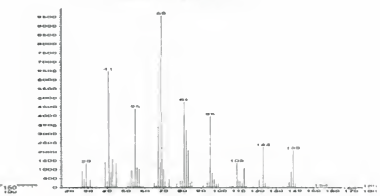
560 3-Mercapto-2-pentanone



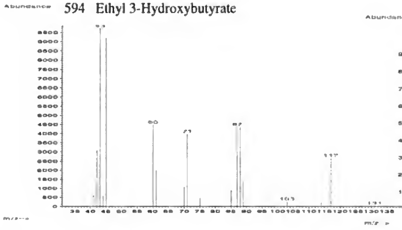
565 Methyl propyl disulfide



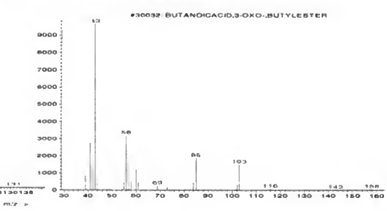
592 Citronelloxyacetaldehyde



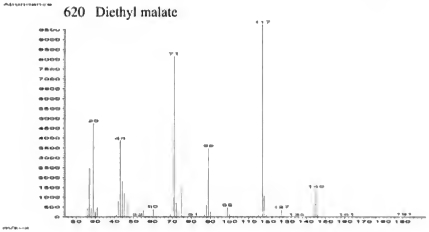
594 Ethyl 3-Hydroxybutyrate



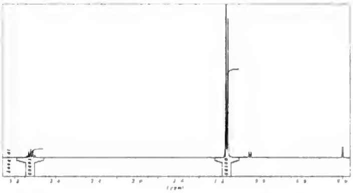
596 Butyl acetoacetate



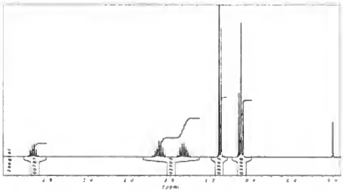
620 Diethyl malate



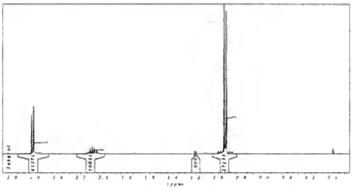
631.1 3-Methyl-2-oxobutanoic acid, sodium



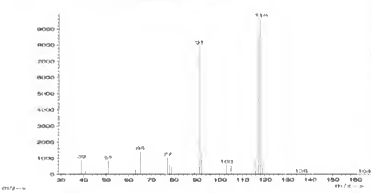
632.1 3-Methyl-2-oxopentanoic acid, sodium



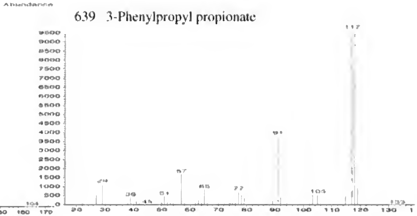
633.1 4-Methyl-2-oxopentanoic acid, sodium



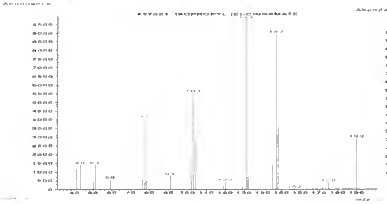
637 3-Phenylpropyl formate



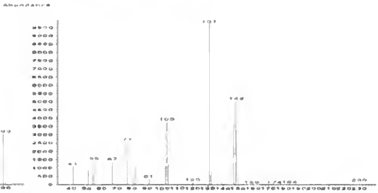
639 3-Phenylpropyl propionate



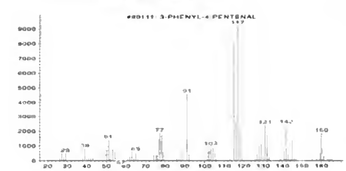
661 Isopropyl cinnamate



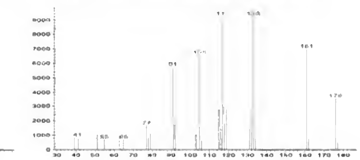
667 Cyclohexyl cinnamate



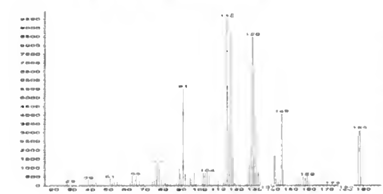
679 3-Phenyl-4-pentenal



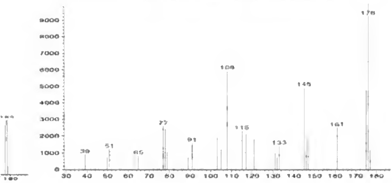
680 3-(p-Isopropylphenyl)propionaldehyde



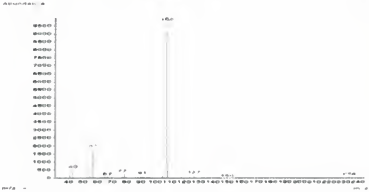
684 alpha-Butylcinnamaldehyde



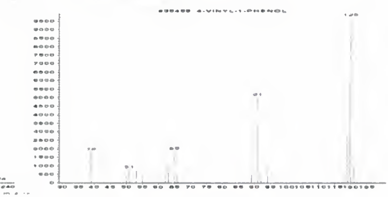
689 p-Methoxy-alpha-methyl-cinnamaldehyde



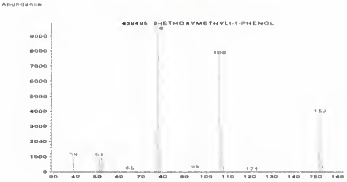
703 p-Tolyl octanoate



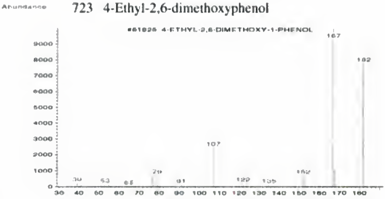
711 p-Vinylphenol



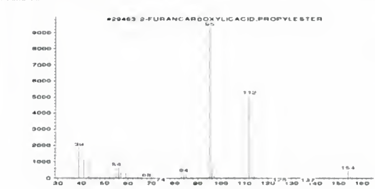
714 o-(Ethoxymethyl)phenol



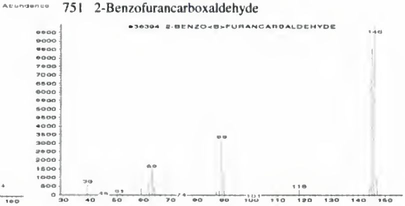
723 4-Ethyl-2,6-dimethoxyphenol



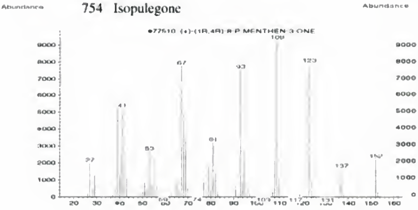
747 Propyl 2-furoate



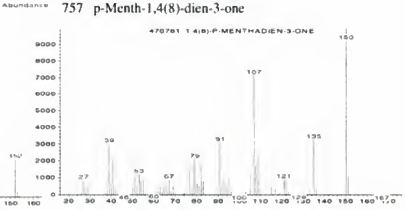
751 2-Benzofurancarboxaldehyde



754 Isopulegone



757 p-Menth-1,4(8)-dien-3-one



Gas Chromatographic (GC) assay of flavouring agents

This procedure applies both to the assay of flavour chemicals and to the quantitation of minor components in flavour chemicals. Analysts following this procedure and performing the test, should obtain sufficient resolution of major and even trace components of a mixture to calculate accurately the concentration of the desired component. They should be familiar with the general principles, usual techniques, and instrumental variables normally met in gas chromatographic analysis. They should pay particular attention to the following:

1. Stability of baseline, return to baseline before and after each peak of interest, and minimum use of recorder attenuation.

2. Any incompatibility between a sensitive sample component and column support, liquid substrate, or construction material.

3. The response to different components of the same or different detectors. Since sizeable errors may be encountered in correlating area percent directly to weight percent, the methods for calculating response factors should be known.

4. Where limits for minor components are specified in the column entitled *Other Requirements* in the above tabular specifications for flavour chemicals, analysts should use authentic materials to confirm the retention times of minor components. Determine the quantity of components following the instructions below under *Calculations and Methods.*

GC CONDITIONS FOR ANALYSIS

Column: open tubular capillary column of fused silica or deactivated glass 30 m long x 0.25 to 0.53 mm id

Stationary phase:

1. For a non-polar column: methyl silicone gum, or equivalent (preferably a bonded and cross-linked dimethyl polysiloxane)

2. For a polar column: polyethylene glycol, or equivalent (preferably a bonded and cross-linked polyethylene glycol)

3. The stationary phase coating should have a thickness of 1 to 3 μm

Carrier gas: helium flowing at a linear velocity of 20 to 40 ml/s

Sample size: 0. 1 to 1.0 μl

Split ratio: (for 0.25 mm to 0.35 mm id columns only) 50:1 to 200:1, typically. Make sure that no individual component exceeds the capacity of the column

Inlet temperature: 225 to 275°

Detector temperature: 250 to 300°

Detectors: use either a thermal conductivity or flame ionization detector operating both as recommended by the manufacturer

Oven program: 50 to 240°, increasing the temperature by 5°/min, hold at 240° for 5 min

Analysts can also use any GC conditions providing separations equal to (or better than) those obtained with the above method, but in the case of a dispute, the above method must stand.

CALCULATIONS AND METHODS

A. Peak area integration with total area detected normalized to 100%, using electronic integrators: Use an electronic peak integrator in accordance with the manufacture's recommendations. Ensure that the integration parameters permit proper integration of the peaks of a variety of shapes and magnitudes and do not interpret baseline shifts and noise spikes as area contributed by the sample. Use internal or external standards as needed to confirm that the total GC peak area corresponds to 100% of the components present in the sample.

B. Results obtained as described above are based on the assumption that the entire sample has eluted and the peaks of all of the components have been included in the calculation. They will be incorrect if any part of the sample does not elute or if all the peaks are not measured. In such cases, and in all methods described above, the internal standard method may be used to determine percentages based on the total sample. For this method, measurements are required of the peaks of the component(s) being assayed and of the internal standard.

An accurately weighed mixture of the internal standard and the sample is prepared and chromatographed, the area ratio(s) of the component(s) to the standard is computed, and the percentage(s) of the component(s) is calculated.

If this calculation is to be applied, the substance used as the standard should be one that meets the following criteria:

a. Its detector response is similar to that of the component(s) to be determined. In general, the more nearly the chemical structure of the component resembles that of the standard, the closer the response will be.

b. Its retention time is close to, but not identical with, that of the component(s).

c. Its elution time is different from that of any other component in the sample so that its peak does not superimpose on any other.

The weight ratio of the internal standard to the sample should be such that the internal standard and the component sought produce approximately equal peaks. This is not possible, of course, if several components of interest are at different levels of concentration.

If the internal standard method is applied properly, it may be assumed that the ratio of the weight of component to the weight of internal standard is exactly proportional to the peak area ratio, and under these conditions no correction factor is needed. The sample is first run by itself to determine whether the internal standard would mask any component by peak superimposition. If there is no interference, a mixture is prepared of the sample and of the internal standard in the specified weight ratio, and the percentages of the internal standard and of the sample in the mixture are calculated. The mixture is chromatographed, and the areas of the component peak and the internal standard peak are calculated by one of the methods described above.

The calculations are as follows:

1.1. % Component in Mixture/ %Internal Standard in Mixture = Component Area/Internal Standard Area, or

1.2. % Component in Mixture = % Internal Standard in Mixture x (Component Area/ Internal Standard Area)

2. % Component in Sample = (%Component in Mixture x 100) / %Sample in Mixture

Should calibration be necessary, mixtures should be prepared of internal standard and component, of either 100% or of known purity. The number of mixtures and the weight ratios to be used depend on the component being analyzed. Usually, three mixtures will be required. The weight ratio of one is chosen so that the heights of component and standard are equal. The ratios of the other two may be two-thirds and four-thirds of their value. Each mixture should be chromatographed at least three times, and areas calculated. The factor for each chromatograph should be calculated as specified below, and the averages taken for each mixture. An overall average factor is calculated from them. The calibration should be performed periodically.

1. Factor = [(Weight of Component x % Purity) / (Weight of Internal Standard x % Purity)] x [(Internal Standard Area) / Component Area]

2. % Component in Sample Mixture = (Component Area x Factor x % Internal Standard in Sample Mixture) / Internal Standard Area

3. % Component in Sample = (% Component in Sample Mixture x 100) / Sample in Sample Mixture

GC SYSTEM SUITABILITY TEST SAMPLE

The GC system suitability test sample consists of an equal-weight mixture of food-quality acetophenone, benzyl alcohol, benzyl acetate, linalool, and hydroxycitronellal.

Using the test sample described below, periodically test the performance of and resolution provided by the gas chromatograph employed. The test sample must display results comparable in quantitative composition, peak shape, and elution order to those specified below. The quantitative composition should not deviate from the results listed below by more than 10%. Analyze the GC test sample using the *GC Conditions for Analysis* given above.

Component in Test Sample	**Order of Elution**		**Normalized % Area (FID)**	
	Non-polar	Polar	Non-polar	Polar
Benzyl alcohol	1	4	22.0	21.3
Acetophenone	2	2	21.1	21.4
Linalool	3	1	20.8	21.0
Benzyl acetate	4	3	18.6	19.1
Hydroxycitronellal	5	5	16.7	16.7

Section C. Principles governing the establishment and revision of specifications

General specifications for enzyme preparations

At its 53rd Session the Committee revised Annex 1 to FNP 52 "General Specifications for Enzyme Preparations Used in Food Processing" (FNP 52 Add 7, Section C) to indicate that only non-toxicogenic and non-pathogenic strains may be used as source organisms in the production of enzyme preparations for use in food.

A number of enzyme preparations were considered at this Session and in each case specific wording was included in the specifications to require that only non-toxicogenic and non-pathogenic strains should be used. As this wording precludes, by definition, the production of toxins, specifications incorporating this wording will normally not require specific limits to be placed on potentially toxic by-products.

Determination of low levels of metals

The Committee continues to pay attention to improving its specifications for limits and methods of analysis of metals. At this meeting, the Committee recognised that in existing monographs where levels of lead of 2 mg/kg or less have been specified, the recommended sample preparation and instrumental methods are not fully satisfactory. In recognition of this problem, the Committee decided to discontinue using the phrase "Prepare a sample solution as directed for organic compounds in the Limit Test and determine by atomic absorption spectroscopy.", and instead to use the wording "Determine using an atomic absorption technique appropriate to the specified level.". The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

This recommendation also applies where low levels for other metals, e.g. cadmium are specified. The Committee agreed that revised sample preparation procedures and instrumental methods should be prepared for consideration at a future meeting and inclusion in FNP 5. Comments and information are invited concerning this matter.

Metals limits for emulsifiers

At its 53rd meeting, the Committee reaffirmed its policy of replacing the outdated test for Heavy Metals (as lead) with limits for individual metals and agreed to begin a programme to implement this policy by calling for proposed levels and supporting data relating to individual metals in emulsifiers for review at the 55th meeting.

Proposed levels and supporting data were received for some organic emulsifiers. On the basis of these data it was decided to delete arsenic specifications and the Heavy Metals (as lead) specifications in these substances and replace them with a lead level of 2 mg/kg, in accordance with the principles stated in FNP 52 Add 7, Section C. Although proposals were also received on the inorganic phosphates listed as having emulsifier use, there were no supporting analytical data. A number of specifications for the phosphate emulsifiers were also amended to change the current limits for arsenic and lead, and to delete limits for Heavy Metals (as lead).

Comments on the proposed limits are invited. Where higher limits are requested, analytical data in support of such limits must be provided. If alternative values and supporting data are not received by 28 February 2001, the proposed metal limits will be considered to supersede the existing metals limits.

In summary, the current limits have been proposed to be changed as follows:

- limits for arsenic were deleted except in the case of phosphates, which were given a proposed arsenic specification of not more than 3 mg/kg
- limits for lead for organic emulsifiers were set at not more than 2 mg/kg and for phosphate emulsifiers at not more than 4 mg/kg
- limits for Heavy Metals (as lead) were deleted

The Committee emphasized that when the Limit Test for Heavy Metals (as lead) is replaced with specifications for individual elements, the absence of a particular metal from a specification means that the level of contamination is so low as to be of no concern.

Proposed metals specifications for 43 emulsifiers

INS	**Additive**	**Arsenic**	**Lead**
		mg/kg	**mg/kg**
472	Acetic acid esters of mono and diglycerides of fatty acids		2
452v	Ammonium polyphosphate	3	4
442	Ammonium salts of phosphatidic acid		2
452iv	Calcium polyphosphate	3	4
482i	Calcium stearoyl-2-lactylate		2
1000	Cholic acid		2
472c	Citric and fatty acid esters acid esters of glycerol		2
	Desoxycholic acid		2
450vi	Dicalcium pyrophosphate (diphosphate)	3	4
480	Dioctyl sodiumsulphosuccinate		2
450i	Disodium pyrophosphate (diphosphate)	3	4
445	Glycerol esters of wood rosin		2
472b	Lactic acid esters of mono and diglycerides of fatty acids		2
322	Lecithin, partially hydrolysed		2
472e,f	Diacetyl tartraric acid esters of glycerol		2
471	Mono and diglycerides of fatty acids		2
475	Polyglycerol esters of fatty acids		2
476	Polyglycerol esters of interesterified ricinoleic acid		2
431	Polyoxyethylene (40) stearate		2
432	Polyoxyethylene sorbitan monolaurate (polysorbate 20)		2
433	Polyoxyethylene sorbitan monooleate (polysorbate 80)		2
434	Polyoxyethylene sorbitan monopalmitate (polysorbate 40)		2
435	Polyoxyethylene sorbitan monostearate (polysorbate 60)		2
436	Polyoxyethylene sorbitan tristearate (polysorbate 65)		2
430	Polyoxyethylene stearate (8)		2
477	Propylene glycol esters of fatty acids		2
470	Salts of fatty acids		2
541ii	Sodium aluminium phosphate, basic	3	4
	Sodium metaphosphate, Insoluble	3	4
452i	Sodium polyphosphate, Glassy	3	4
481i	Sodium stearoyl-2-lactylate		2
494	Sorbitan monooleate		2
495	Sorbitan monopalmitate		2
491	Sorbitan monostearate		2
492	Sorbitan tristearate		2
484	Stearyl citrate		2
	Stearyl monoglceridyl citrate		2
472g	Succinylated monoglycerides		2
474	Sucroglycerides		2
450v	Tetra potassium pyrophosphate	3	4
450iii	Tetra sodium pyrophosphate	3	4
	Thermally oxidised soya bean oil		2
479b	Thermally oxidized soya bean oil/ glycerides of fatty acids		2

INS: International Numbering System

Tentative specifications for food additives (uses other than as flavouring agent)

At the 53rd JECFA the Committee noted that many of the specifications for food additives published in the FAO Compendium of Food Additives (FNP 52) and its Addenda were designated as "tentative", indicating that some data were missing or incomplete at the time the specifications were prepared. For the current meeting, no responses to the call for data for several of these compounds were received and consequently their tentative specifications were withdrawn. These compounds are: acetone peroxides, aluminum sodium sulfate, ammonium persulfate, benzoin gum, calcium iodate, calcium peroxide, carbohydrase from *Aspergillus niger*, var., carbohydrase from *Aspergillus awamori*, var., chlorine dioxide, isoamyl gallate, lipase from *Aspergillus oryzae*, var., 2-nitropropane, potassium persulfate, rennet from *Endothia parasitica*, and trichloroethylene.

Information was received for aluminium potassium sulfate, aluminium sulfate (anhydrous), ammonium salts of phosphatidic acid, diatomaceous earth and rennet from *Mucor* species. Their specifications were revised and the tentative designations were deleted. The title for rennet from *Mucor* species was changed to rennet from *Rhizomucor* species to reflect the new classification of the source organisms.

The tentative specifications of diethyl pyrocarbonate were withdrawn because this compound was considered by the 17th JECFA (1973) to be unacceptable for use in foods.

Tentative specifications for flavouring agents

The call for data for the 55th Session included requests for information on

- the 284 specifications developed at the 49th , 51st and 53rd Sessions, which were assigned tentative specifications at the 53rd Session
- 59 non-tentative specifications for which the minimum assay figure was less than 95%
- proposed specifications for a further 124 flavourings to be considered for the first time at the current Session.

The information provided in response to the request for additional information on the specifications developed at the 49th, 51st and 53rd Sessions (1996-99) permitted the Committee to assign a full status to a further 179 specifications previously designated as tentative. However the Committee noted that data were provided for only 3 of the 59 flavourings for which data were requested on the minimum assay values.

The Committee reaffirmed that these data were needed in order to establish satisfactory specifications, and agreed that the 56 specifications for which data were still lacking should be reclassified as tentative pending receipt of this information.

As a result of the above considerations, 476 out of 637 specifications from 1996-9 (75%) were classified as "full", and 161 out of 637 specifications (25%) were classified as "tentative".

At its 53rd Session the Committee indicated that unless the missing information was provided for those substances with a tentative designation, and those for which the minimum assay figures were less than 95%, the specifications would be withdrawn. In the light of the good response from industry in providing data on the tentative specifications the Committee decided to relax this requirement although, as indicated below, it stressed that the missing data on all the specifications developed to date must now be provided in time for consideration at the Committee's meeting in 2001.

The Committee noted that the information provided for the 55th Session to be considered for the first time was much more complete than in the past and this resulted in most of the flavours being assigned full specifications. In addition most of the missing information on the earlier (1996-99) specifications has now been provided. However a significant number of tentative specifications remain in both the 1996-99 lists and in the list of substances first considered at this meeting. The Committee stresses that the data necessary to enable these specifications to be given a full status need to be provided in time for consideration by the 57th Session due to be held in 2001.

The Committee also noted that the information on the nature of the products often did not make it clear which particular isomers were present. Unless more specific information is provided on the isomers present in individual flavourings, the Committee will proceed on the assumption that all the possible isomers may be present.

FAO TECHNICAL PAPERS

FAO FOOD AND NUTRITION PAPERS

1/1	Review of food consumption surveys 1977 – Vol. 1. Europe, North America, Oceania, 1977 (E)
1/2	Review of food consumption surveys 1977 – Vol. 2. Africa, Latin America, Near East, Far East, 1979 (E)
2	Report of the joint FAO/WHO/UNEP conference on mycotoxins, 1977 (E F S)
3	Report of a joint FAO/WHO expert consultation on dietary fats and oils in human nutrition, 1977 (E F S)
4	JECFA specifications for identity and purity of thickening agents, anticaking agents, antimicrobials, antioxidants and emulsifiers, 1978 (E)
5	JECFA – guide to specifications, 1978 (E F)
5 Rev. 1	JECFA – guide to specifications, 1983 (E F)
5 Rev. 2	JECFA – guide to specifications, 1991 (E)
6	The feeding of workers in developing countries, 1976 (E S)
7	JECFA specifications for identity and purity of food colours, enzyme preparations and other food additives, 1978 (E F)
8	Women in food production, food handling and nutrition, 1979 (E F S)
9	Arsenic and tin in foods: reviews of commonly used methods of analysis, 1979 (E)
10	Prevention of mycotoxins, 1979 (E F S)
11	The economic value of breast-feeding, 1979 (E F)
12	JECFA specifications for identity and purity of food colours, flavouring agents and other food additives, 1979 (E F)
13	Perspective on mycotoxins, 1979 (E F S)
14	*Manuals of food quality control:*
14/1	Food control laboratory, 1979 (Ar E)
14/1 Rev.1	The food control laboratory, 1986 (E)
14/2	Additives, contaminants, techniques, 1980 (E)
14/3	Commodities, 1979 (E)
14/4	Microbiological analysis, 1979 (E F S)
14/5	Food inspection, 1981 (Ar E) (Rev. 1984, E S)
14/6	Food for export, 1979 (E S)
14/6 Rev.1	Food for export, 1990 (E S)
14/7	Food analysis: general techniques, additives, contaminants and composition, 1986 (C E)
14/8	Food analysis: quality, adulteration and tests of identity, 1986 (E)
14/9	Introduction to food sampling, 1988 (Ar C E F S)
14/10	Training in mycotoxins analysis, 1990 (E S)
14/11	Management of food control programmes, 1991 (E)
14/12	Quality assurance in the food control microbiological laboratory, 1992 (E F S)
14/13	Pesticide residue analysis in the food control laboratory, 1993 (E F)
14/14	Quality assurance in the food control chemical laboratory, 1993 (E)
14/15	Imported food inspection, 1993 (E F)
14/16	Radionuclides in food, 1994 (E)
14/17	Unacceptable visible can defects – a pictorial manual, 1998 (E F S)
15	Carbohydrates in human nutrition, 1980 (E F S)
16	Analysis of food consumption survey data for developing countries, 1980 (E F S)
17	JECFA specifications for identity and purity of sweetening agents, emulsifying agents, flavouring agents and other food additives, 1980 (E F)
18	Bibliography of food consumption surveys, 1981 (E)
18 Rev. 1	Bibliography of food consumption surveys, 1984 (E)
18 Rev. 2	Bibliography of food consumption surveys, 1987 (E)
18 Rev. 3	Bibliography of food consumption surveys, 1990 (E)
19	JECFA specifications for identity and purity of carrier solvents, emulsifiers and stabilizers, enzyme preparations, flavouring agents, food colours, sweetening agents and other food additives, 1981 (E F)
20	Legumes in human nutrition, 1982 (E F S)
21	Mycotoxin surveillance – a guideline, 1982 (E)
22	Guidelines for agricultural training curricula in Africa, 1982 (E F)
23	Management of group feeding programmes, 1982 (E F P S)
23 Rev. 1	Food and nutrition in the management of group feeding programmes, 1993 (E F S)
24	Evaluation of nutrition interventions, 1982 (E)
25	JECFA specifications for identity and purity of buffering agents, salts; emulsifiers, thickening agents, stabilizers; flavouring agents, food colours, sweetening agents and miscellaneous food additives, 1982 (E F)
26	Food composition tables for the Near East, 1983 (E)
27	Review of food consumption surveys 1981, 1983 (E)
28	JECFA specifications for identity and purity of buffering agents, salts, emulsifiers, stabilizers, thickening agents, extraction solvents, flavouring agents, sweetening agents and miscellaneous food additives, 1983 (E F)
29	Post-harvest losses in quality of food grains, 1983 (E F)
30	FAO/WHO food additives data system, 1984 (E)
30 Rev. 1	FAO/WHO food additives data system, 1985 (E)
31/1	JECFA specifications for identity and purity of food colours, 1984 (E F)
31/2	JECFA specifications for identity and purity of food additives, 1984 (E F)
32	Residues of veterinary drugs in foods, 1985 (E/F/S)
33	Nutritional implications of food aid: an annotated bibliography, 1985 (E)
34	JECFA specifications for identity and purity of certain food additives, 1986 (E F)
35	Review of food consumption surveys 1985, 1986 (E)
36	Guidelines for can manufacturers and food canners, 1986 (E)
37	JECFA specifications for identity and purity of certain food additives, 1986 (E F)
38	JECFA specifications for identity and purity of certain food additives, 1988 (E)
39	Quality control in fruit and vegetable processing, 1988 (E F S)
40	Directory of food and nutrition institutions in the Near East, 1987 (E)
41	Residues of some veterinary drugs in animals and foods, 1988 (E)
41/2	Residues of some veterinary drugs in animals and foods. Thirty-fourth meeting of the joint FAO/WHO Expert Committee on Food Additives, 1990 (E)
41/3	Residues of some veterinary drugs in animals and foods. Thirty-sixth meeting of the joint FAO/WHO Expert Committee on Food Additives, 1991 (E)
41/4	Residues of some veterinary drugs in animals and foods. Thirty-eighth meeting of the joint FAO/WHO Expert Committee on Food Additives, 1991 (E)

41/5 Residues of some veterinary drugs in animals and foods. Fortieth meeting of the Joint FAO/WHO Expert Committee on Food Additives, 1993 (E)

41/6 Residues of some veterinary drugs in animals and foods. Forty-second meeting of the Joint FAO/WHO Expert Committee on Food Additives, 1994 (E)

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41/9 Residues of some veterinary drugs in animals and foods. Forty-seventh meeting of the Joint FAO/WHO Expert Committee on Food Additives, 1997 (E)

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Availability: November 2000

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This document is one of the three publications prepared by the fifty-fifth session of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), held in Geneva, Switzerland, in June 2000, and dedicated to the evaluation of food additives and contaminants in food.

The report of the meeting will be published in the WHO Technical Report Series and the toxicological monographs as No. 46 in the WHO Food Additives Series. Specifications of certain food additives in this document provide information on their identity and purity. The three main objectives of these specifications are to identify the substance that has been subject to biological testing, to ensure that the substance is of the quality required for safe use in food and to reflect and encourage good manufacturing practice (GMP). This publication will be useful to all who work with or are interested in food additives and their safe use in food.

ISBN 92-5-104508-9 ISSN 0254-4725
9 789251 045084
TC/M/X8562E/1/10 00/2260